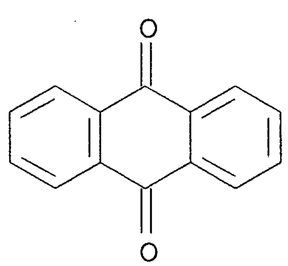
=> d l48 1-12 cbib abs hitstr hitind

L48 ANSWER 1 OF 12 HCA COPYRIGHT 2003 ACS
136:56010 Process for **manufacture** of **hydrogen peroxide** and composition for use therein. Nystroem, Mats; Jaernvik, Christina (Akzo Nobel N.V., Neth.; Eka Chemicals AB). PCT Int. Appl. WO 2001098204 A1 20011227, 10 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-SE1192 20010528. PRIORITY: EP 2000-850109 20000619; US 2000-PV212633 20000619.

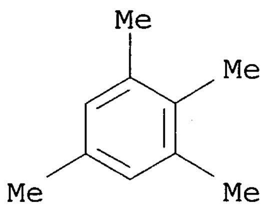
AB The invention relates to a process for **prodn**. of **hydrogen peroxide** according to the **anthraquinone** process including alternate hydrogenation and oxidn. of one or more **quinones** selected from **anthraquinones** and/or **tetrahydro anthraquinones** in a working soln. comprising at least one **quinone** solvent and at least one **hydroquinone** solvent, wherein said at least one **quinone** solvent comprises **isodurene** in an amt. from 15 wt.% to 100 wt%. The invention also relates to a compn. useful as a working soln. at **prodn**. of **hydrogen peroxide**.

IT **84-65-1**, 9,10-Anthracenedione **527-53-7** **28758-94-3**
(process for **manuf**. of **hydrogen peroxide** and compn. for use therein)

RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



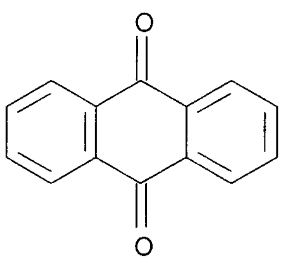
RN 527-53-7 HCA
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 28758-94-3 HCA
CN 9,10-Anthracenedione, tetrahydro- (9CI) (CA INDEX NAME)

CM 1

CRN 84-65-1
CMF C14 H8 O2



IT **7722-84-1P, Hydrogen peroxide, preparation**
(process for **manuf**. of **hydrogen peroxide** and compn. for use therein)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

IC ICM C01B015-023
CC 49-8 (Industrial Inorganic Chemicals)
ST **hydrogen peroxide manuf anthraquinone** process
IT Hydrogenation
Oxidation
Solvents
(process for **manuf**. of **hydrogen peroxide** and compn. for use therein)
IT **Quinones**
(process for **manuf**. of **hydrogen peroxide** and compn. for use therein)
IT **84-65-1**, 9,10-Anthracenedione 108-82-7 **527-53-7**
4559-86-8 **28758-94-3**

(process for **manuf**. of **hydrogen peroxide** and compn. for use therein)

IT **7722-84-1P, Hydrogen peroxide, preparation**
(process for **manuf**. of **hydrogen peroxide** and compn. for use therein)

L48 ANSWER 2 OF 12 HCA COPYRIGHT 2003 ACS

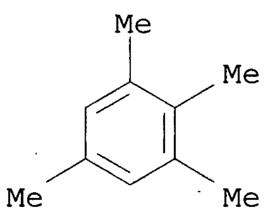
136:45554 Efficient Catalysis of Rare-Earth Metal Ions in Photoinduced Electron-Transfer Oxidation of Benzyl Alcohols by a Flavin Analogue. Fukuzumi, Shunichi; Yasui, Kiyomi; Suenobu, Tomoyoshi; Ohkubo, Kei; Fujitsuka, Mamoru; Ito, Osamu (Department of Material and Life Science Graduate School of Engineering, Osaka University CREST Japan Science and Technology Corporation (JST), Suita Osaka, 565-0871, Japan). Journal of Physical Chemistry A, 105(46), 10501-10510 (English) 2001. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB A flavin analog (riboflavin-2',3',4',5'-tetraacetate, Fl) forms the 1:1 and 1:2 complexes with rare-earth metal ions. The largest formation consts. K1 and K2 for the 1:1 and 1:2 complexes between Fl and Sc3+ are detd. as K1 = 3.1 .times. 104 M-1 and K2 = 1.4 .times. 103 M-1, resp. The complexation of Fl with rare-earth metal ions results in blue shifts of the fluorescence max., shortening of the fluorescence lifetime, and more importantly the change in the lowest excited state from the n,.pi.* triplet state of Fl to the .pi.,.pi.* singlet states of Fl-rare-earth metal ion complexes as indicated by the disappearance of the triplet-triplet (T-T) absorption spectrum of Fl by the complexation with metal ions. The strong complex formation between Fl and rare-earth metal ions enhances the oxidizing ability of the excited state of Fl as indicated by the significant acceleration in the fluorescence quenching rates of Fl-rare earth metal ion complexes via electron transfer from electron donors (e.g., alkylbenzenes) as compared to those of uncomplexed Fl. The one-electron redn. potential of the singlet excited state of the 1:2 complex between Fl and Sc3+, 1(Fl-2Sc3+)* is pos. shifted by 780 mV as compared to 1Fl*. Such a remarkable enhancement of the redox reactivity of 1(Fl-2Sc3+)* as compared to that of 1Fl* makes it possible to oxidize efficiently p-chlorobenzyl alc. to p-chlorobenzaldehyde by 1(Fl-2Sc3+)*, although no photooxidn. of p-chlorobenzyl alc. by Fl occurred in deaerated MeCN. The quantum yield for the photooxidn. of p-chlorobenzyl alc. by Fl-2Sc3+ is the largest among various Fl-metal ion complexes. A comparison of the obsd. rate const. derived from the dependence of the quantum yield on the concn. of p-chlorobenzyl alc. with the fluorescence quenching rate const. by electron transfer from the alc. and the direct detection of radical intermediates reveal that the photooxidn. proceeds via electron transfer from p-chlorobenzyl alc. to 1(Fl-2Sc3+)*. Under an atm. pressure of oxygen, the photooxidn. of p-methoxybenzyl alc. by oxygen proceeds efficiently in the presence of Fl-Lu3+ which acts as an efficient photocatalyst. No photodegrdn. was obsd. in the case of the Fl-Lu3+ complex, whereas the facile photodegrdn. of Fl-Mg2+ has precluded the

efficient photocatalytic oxidn. of the alc. by oxygen.
IT **7722-84-1**, **Hydrogen peroxide**, properties
(photoproduct; electron-transfer photooxidn. of benzyl alcs. catalyzed by rare-earth ion complexes of riboflavin tetraacetate)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

IT **527-53-7**, 1,2,3,5-Tetramethylbenzene
(quencher; kinetics of fluorescence quenching of riboflavin tetraacetate by benzene derivs. in presence and absence of rare earth metal ions)
RN 527-53-7 HCA
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 22
IT 104-88-1, p-Chlorobenzaldehyde, properties 123-11-5, p-Methoxybenzaldehyde, properties **7722-84-1**, **Hydrogen peroxide**, properties
(photoproduct; electron-transfer photooxidn. of benzyl alcs. catalyzed by rare-earth ion complexes of riboflavin tetraacetate)
IT 95-47-6, o-Xylene, properties 95-63-6, 1,2,4-Trimethylbenzene 99-87-6, p-Cymene 100-41-4, Ethylbenzene, properties 106-42-3, p-Xylene, properties 108-38-3, properties 108-88-3, Toluene, properties 151-10-0 488-23-3, 1,2,3,4-Tetramethylbenzene 526-73-8, 1,2,3-Trimethylbenzene **527-53-7**, 1,2,3,5-Tetramethylbenzene 700-12-9, Pentamethylbenzene
(quencher; kinetics of fluorescence quenching of riboflavin tetraacetate by benzene derivs. in presence and absence of rare earth metal ions)

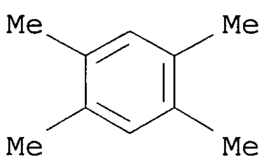
L48 ANSWER 3 OF 12 HCA COPYRIGHT 2003 ACS
128:270417 Selective C-H bond activation of arenes catalyzed by methylrhenium trioxide. Jacob, Josemon; Espenson, James H. (Ames Laboratory and Department of Chemistry, Iowa State University, Ames, IA, 50011, USA). Inorganica Chimica Acta, 270(1,2), 55-59 (English) 1998. CODEN: ICHAA3. ISSN: 0020-1693. OTHER SOURCES: CASREACT 128:270417. Publisher: Elsevier Science S.A..
AB Arenes, in glacial acetic acid, are oxidized to p-benzoquinones by

hydrogen peroxide when methylrhenium trioxide (CH_3ReO_3 or MTO) is used as a catalyst. In some cases an intermediate hydroquinone was also obtained in lower yield. Oxidn. of the Me side chains of various methylbenzenes did not occur. The active catalyst species are the previously characterized .eta.2-peroxorhenium complexes, CH3Re(O)2(.eta.2-O2) and CH3Re(O)(.eta.2-O2)2(H2O). Sep. tests showed that hydroquinones and phenols are oxidized by **H2O2**-MTO more rapidly than the simple arenes; in the proposed mechanism they are intermediate products. Higher conversions were found for the more highly-substituted arenes, consistent with their being the most reactive species toward the electrophilically active peroxide bound to rhenium. High conversions of the less substituted members of the series were not achieved, reflecting concurrent deactivation of MTO-peroxide, a process of greater import for the more slowly reacting substrates.

IT **95-93-2**, 1,2,4,5-Tetramethylbenzene
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 85-01-8, Phenanthrene, reactions 95-47-6, o-Xylene, reactions 95-48-7, 2-Methylphenol, reactions 95-63-6, 1,2,4-Trimethylbenzene **95-93-2**, 1,2,4,5-Tetramethylbenzene 106-42-3, p-Xylene, reactions 108-38-3, reactions 119-64-2, Tetralin 120-12-7, Anthracene, reactions
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

IT 84-11-7P, **Phenanthraquinone** 84-65-1P, **Anthraquinone** 137-18-8P, 2,5-Dimethyl-p-benzoquinone 526-86-3P, 2,3-Dimethyl-p-benzoquinone 527-17-3P, Tetramethyl-p-benzoquinone 527-61-7P, 2,6-Dimethyl-p-benzoquinone 553-97-9P, Methyl-p-benzoquinone 935-92-2P, Trimethyl-p-benzoquinone 7474-90-0P
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

L48 ANSWER 4 OF 12 HCA COPYRIGHT 2003 ACS

117:197698 Investigation on chemical/physical treatment of leachate of hazardous waste landfill. Foerst, C.; Stieglitz, L.; Barth, H. (Kernforschungszent. Karlsruhe, Karlsruhe, D-7500/1, Germany). Altlastensanierung 90, Int. KfK/TNO Kongr., 3rd, Meeting Date 1990, 1229-36. Editor(s): Arendt, Friedrich; Hinsenveld, M.; Van den

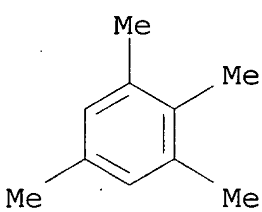
Brink, W. J. Bundesminist. Forsch. Technol.: Bonn, Germany. (German) 1991. CODEN: 57ZNA6.

AB The concns. of most organochlorine and alkylbenzene contaminants in mock landfill leachate samples were decreased by 50-90% by oil removal, with the exception of 2,4- and 2,5-dichlorophenols. Removal of most of these substances was 95-100% complete (to sub-ppb levels) after flocculation and pptn., provided that **H2O2** was added to oxidize Fe2+; the best results were obtained at pH >8.5. Removal of 2,4- and 2,5-dichlorophenols was still only 82% complete under these conditions. Org. C, Fe, and Ca were decreased by >50, 90, and 70%, resp., after flocculation and pptn.

IT **527-53-7**, 1,2,3,5-Tetramethylbenzene
(removal of, from landfill leachate, by oil removal and oxidn.-flocculation-pptn.)

RN 527-53-7 HCA

CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)

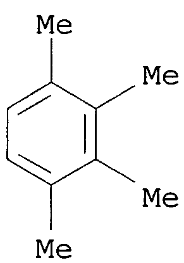


CC 60-2 (Waste Treatment and Disposal)

IT 58-89-9, .gamma.-HCH 67-66-3, Chloroform, miscellaneous 71-43-2, Benzene, miscellaneous 71-43-2D, Benzene, alkyl derivs. 71-55-6, 1,1,1-Trichloroethane 75-09-2, Dichloromethane, miscellaneous 75-35-4, 1,1-Dichloroethene, miscellaneous 79-01-6, Trichloroethene, miscellaneous 87-61-6, 1,2,3-Trichlorobenzene 87-65-0, 2,6-Dichlorophenol 88-06-2, 2,4,6-Trichlorophenol 95-47-6, o-Xylene, miscellaneous 95-50-1, o-Dichlorobenzene 95-63-6, 1,2,4-Trimethylbenzene 95-77-2, 3,4-Dichlorophenol 95-93-2, 1,2,4,5-Tetramethylbenzene 95-94-3, 1,2,4,5-Tetrachlorobenzene 95-95-4, 2,4,5-Trichlorophenol 100-41-4, Ethylbenzene, miscellaneous 103-65-1, Propylbenzene 106-42-3, p-Xylene, miscellaneous 106-46-7, p-Dichlorobenzene 107-06-2, 1,2-Dichloroethane, miscellaneous 108-38-3, m-Xylene, miscellaneous 108-67-8, 1,3,5-Trimethylbenzene, miscellaneous 108-70-3, 1,3,5-Trichlorobenzene 108-88-3, Toluene, miscellaneous 108-90-7, Chlorobenzene, miscellaneous 120-82-1, 1,2,4-Trichlorobenzene 120-83-2, 2,4-Dichlorophenol 127-18-4, Tetrachloroethene, miscellaneous 156-59-2, cis-1,2-Dichloroethene 319-84-6, .alpha.-HCH 319-86-8, .delta.-HCH 488-23-3, 1,2,3,4-Tetramethylbenzene 526-73-8, 1,2,3-Trimethylbenzene **527-53-7**, 1,2,3,5-Tetramethylbenzene 541-73-1, m-Dichlorobenzene 583-78-8, 2,5-Dichlorophenol 591-35-5, 3,5-Dichlorophenol 608-93-5, Pentachlorobenzene 634-66-2, 1,2,3,4-Tetrachlorobenzene 634-90-2, 1,2,3,5-Tetrachlorobenzene 7439-89-6, Iron, miscellaneous 7440-70-2, Calcium, miscellaneous

(removal of, from landfill leachate, by oil removal and oxidn.-flocculation-pptn.)

L48 ANSWER 5 OF 12 HCA COPYRIGHT 2003 ACS
115:123516 Chemiluminescent systems. Essenfeld, Amy P.; Freeman, John J. (American Cyanamid Co., USA). Eur. Pat. Appl. EP 429863 A2 19910605, 5 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1990-120660 19901029. PRIORITY: US 1989-443618 19891130.
AB The use of 1,2,4-trimethyl-9,10-bis(phenylethenyl)anthracene or 1,2,3,4-tetramethyl-9,10-bis(phenylethynyl)anthracene as a fluorescer component in **H2O2**-oxalate ester-fluorescer chemiluminescent systems, and the compds. themselves, are claimed.
IT **488-23-3**, 1,2,3,4-Tetramethylbenzene
(reaction of, in chemiluminescent fluorescer prepn.)
RN 488-23-3 HCA
CN Benzene, 1,2,3,4-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IC ICM C09K011-07
CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 25
IT 95-63-6, 1,2,4-Trimethylbenzene **488-23-3**, 1,2,3,4-Tetramethylbenzene 20153-30-4, 1,2,4-**Trimethylanthraquinone**
(reaction of, in chemiluminescent fluorescer prepn.)

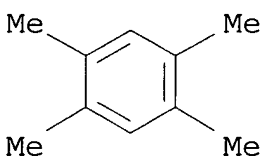
L48 ANSWER 6 OF 12 HCA COPYRIGHT 2003 ACS
112:35397 Oxidation of methoxy- and/or methyl-substituted benzenes and naphthalenes to quinones and phenols by **hydrogen peroxide** in **formic** acid. Orita, Hideo; Shimizu, Masao; Hayakawa, Takashi; Takehira, Katsuomi (Natl. Chem. Lab. Ind., Tsukuba, 305, Japan). Bulletin of the Chemical Society of Japan, 62(5), 1652-7 (English) 1989. CODEN: BCSJA8. ISSN: 0009-2673. OTHER SOURCES: CASREACT 112:35397.
AB The oxidn. of a no. of arenes (methoxybenzenes, methylbenzenes, and d naphthalenes) to quinones and phenols by H2O2 in HCO2H has been examd. Methoxybenzenes were much more easily oxidized to p-benzoquinones than methylbenzenes (e.g., 1,3,5-trimethoxybenzene was oxidized to 2,6-dimethoxy-p-benzoquinone in a 75% yield and 1,2,4-trimethylbenzene to 2,3,5-trimethyl-p-benzoquinone in a 16%

yield). Electron-withdrawing substituents, such as nitro, cyano, and chloro groups, lowered the conversion of reactants and changed the product selectivity from quinones to phenols. Methoxybenzonitriles were oxidized to corresponding phenols in a moderate yield (e.g., 2,6-dimethoxybenzonitrile to 3-hydroxy-2,6-dimethoxybenzonitrile in a 39% yield and a 64% selectivity).

IT **95-93-2**
(oxidn. of, with **hydrogen peroxide** in **formic** acid)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Oxidation
(of methoxy(methyl)benzene with **hydrogen peroxide** in **formic** acid)

IT 91-20-3, Naphthalene, reactions 91-57-6, 2-Methylnaphthalene 95-63-6, 1,2,4-Trimethylbenzene **95-93-2** 100-84-5, m-Methoxytoluene 104-47-2 104-93-8, p-Methoxytoluene 106-42-3, 1,4-Dimethylbenzene, reactions 135-77-3, 1,2,4-Trimethoxybenzene 150-78-7, 1,4-Dimethoxybenzene 494-99-5, 3,4-Dimethoxytoluene 578-58-5, o-Methoxytoluene 581-40-8, 2,3-Dimethylnaphthalene 621-23-8, 1,3,5-Trimethoxybenzene 634-36-6, 1,2,3-Trimethoxybenzene 642-71-7 4107-65-7, 2,4-Dimethoxybenzonitrile 4179-19-5, 3,5-Dimethoxytoluene 4463-33-6, 2,3-Dimethoxytoluene 5150-42-5, 2,3-Dimethoxyquinone 5673-07-4, 2,6-Dimethoxytoluene 6443-69-2, 3,4,5-Trimethoxytoluene 14107-97-2, 2,4,6-Trimethoxytoluene 16932-49-3, 2,6-Dimethoxybenzonitrile 19179-31-8 38064-90-3, 2,4-Dimethoxytoluene
(oxidn. of, with **hydrogen peroxide** in **formic** acid)

L48 ANSWER 7 OF 12 HCA COPYRIGHT 2003 ACS

89:26941 **Hydrogen peroxide**. Giesselmann, Guenter; Schreyer, Gerd; Wagner, Rudolf (Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler, Fed. Rep. Ger.). S. African ZA 7605600 19770823, 14 pp. (English). CODEN: SFXXAB. APPLICATION: ZA 1976-5600 19760917.

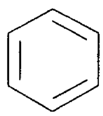
AB For the **anthraquinone** process to **produce H2O2**, mixts. of compds. in the working soln. can be selected for higher capacities without danger from excessive **H2O2** concns. A recycle soln. compn. of 100 g 2-**ethylanthraquinone**, 100 g 2-**ethyltetrahydroanthraquinone**, 0.7 L tetramethylbenzene mixt., 0.15 L trioctyl phosphate,

and 0.15 L N,N-diethyl-N',N'-di-n-butylurea had a capacity of 15 g **H2O2**/L of recycle soln.

IT **25619-60-7**
(in **hydrogen peroxide manuf**., with **alkylanthraquinone** mixts.)

RN 25619-60-7 HCA

CN Benzene, tetramethyl- (8CI, 9CI) (CA INDEX NAME)



4 (D1—Me)

IT **7722-84-1P**, preparation
(manuf. of, **alkylanthraquinone** mixt. in)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO—OH

IC C07C

CC 49-8 (Industrial Inorganic Chemicals)

ST **hydrogen peroxide anthraquinone** process

IT 84-51-5 28555-16-0
(**hydrogen peroxide manuf**. by **alkylanthraquinone** mixts. contg.)

IT 1806-54-8 **25619-60-7** 36654-90-7
(in **hydrogen peroxide manuf**., with **alkylanthraquinone** mixts.)

IT **7722-84-1P**, preparation
(manuf. of, **alkylanthraquinone** mixt. in)

L48 ANSWER 8 OF 12 HCA COPYRIGHT 2003 ACS

63:54365 Original Reference No. 63:9861b-c Isomerization of alkyl aromatics. (Engelhard Industries, Inc.). GB 994123 19650602, 8 pp. (Unavailable). APPLICATION: GB 19631004.

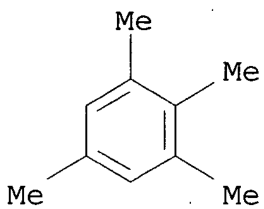
AB A process for the isomerization of C8-10 alkylbenzenes by heating in the presence of H and a catalyst consisting of Al2O3, B2O3, and a noble metal is described. Calcined Pt-Al2O3 catalyst (Brit. 735,390) was stirred with a soln. of 50 g. H3BO3 in 279 ml. deionized **H2O2**, the mixt. dried at 284.degree.F. 4 hrs in a stream of air, and heated at 1000.degree.F. for 2 hrs. The isomerization app. for continuous operation was charged with 88 g. catalyst and H passed through at 0.5-1.0 ft.2/hr. while feeding in the aromatic mixt. In an example, a mixt. of PhEt 4.2, o-C6H4Me2

(I) 0.5, m-C6H4Me2 (II), 92.8, p-C6H4Me2 (III) 1.2, and 1% paraffins + olefins + naphthenes 1% treated at 800.degree.F. and 175 psig. gave a product consistent of paraffins 7, PhEt 5.4, I 18.2, II 38.6, III 17.8, C6H6 0.5, PhMe 3.6, C9+ aromatics 5.1, and C+6 naphthenes 3.5%.

IT **527-53-7**, Benzene, 1,2,3,5-tetramethyl-
(isomerization of, catalysis by Al2O3-B2O3-Pt)

RN 527-53-7 HCA

CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IC C07C

CC 35 (Noncondensed Aromatic Compounds)

IT 108-38-3, m-Xylene **527-53-7**, Benzene, 1,2,3,5-tetramethyl-
(isomerization of, catalysis by Al2O3-B2O3-Pt)

L48 ANSWER 9 OF 12 HCA COPYRIGHT 2003 ACS

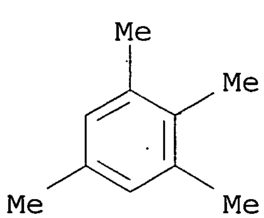
59:53766 Original Reference No. 59:9701d-e Investigation of monocyclic aromatic hydrocarbons of the kerosine from the Minnibaevsk crude oil by ultraviolet absorption spectroscopy. Mukhamedova, L. A.; Baiburova, M. Kh. Izv. Kazansk. Filiala Akad. Nauk. SSSR, Ser. Khim. Nauk (6), 87-92 (Unavailable) 1961.

AB The title compds. were isolated from a kerosine fraction b. 200-300.degree. by chromatography on SiO2 and Al2O3, removal of S compds. with **H2O2**, distn. into 5.degree. fractions, and purification as picrates. The ultraviolet spectral analysis showed the presence of m- and p-dialkylbenzenes. No ortho isomers were found. All isomeric tetramethylbenzenes were present.

IT **527-53-7**, Benzene, 1,2,3,5-tetramethyl-
(in kerosine fraction of Minnibaevsk petroleum)

RN 527-53-7 HCA

CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)

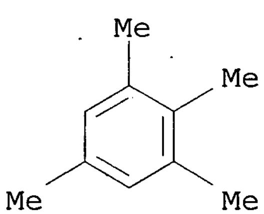


CC 27 (Petroleum and Petroleum Derivatives)

IT 95-93-2, Benzene, 1,2,4,5-tetramethyl- 488-23-3, Benzene,

1,2,3,4-tetramethyl- **527-53-7**, Benzene,
1,2,3,5-tetramethyl-
(in kerosine fraction of Minnibaevsk petroleum)

L48 ANSWER 10 OF 12 HCA COPYRIGHT 2003 ACS
59:48020 Original Reference No. 59:8631g-h,8632a Peroxytrifluoroacetic acid-boron fluoride as a source of positive hydroxyl. Buehler, Charles A.; Hart, Harold (Michigan State Univ., East Lansing). Journal of the American Chemical Society, 85(14), 2177-8 (Unavailable) 1963. CODEN: JACSAT. ISSN: 0002-7863.
GI For diagram(s), see printed CA Issue.
AB To a soln. of 56.1 g. (0.468 mole) mesitylene (I) in 100 ml. CH2Cl2 (II) was added peroxytrifluoroacetic acid (III), prepd. from 35 g. (0.167 mole) trifluoroacetic anhydride, 50 ml. II, and 4 ml. (0.148 mole) 90%, **H2O2**. BF3 was bubbled through the reaction mixt. during the addn. which took 2.5 hrs. The reaction was strongly exothermic and the temp. was kept below 7.degree. by external cooling. H2O was added, the org. layer washed with bisulfite and bicarbonate, dried, and distd. to give 32.0 g. I and 17.7 g. (88% yield) mesitol, m. 69-70.degree.. Similarly, **isodurene** gave isodurenol in 62% yield. Extension of the reaction to prehnitene gave 9% 2,3,4,5-tetramethylphenol, 3.6% 2,3,4,6-tetramethylphenol, 1.8% 2,2,3,4-tetramethylcyclohexa-3,5-dienone, and the major products, 2,3,5- and 2,3,6-trimethylphenol and IV. V was the major product from the reaction of III with chloromesitylene. Nitromesitylene gave a product similar to V. A mechanism was suggested for the reaction of prehnitene with III.
IT **527-53-7**, Benzene, 1,2,3,5-tetramethyl-
(oxidn. by BF3-F3CCO3H)
RN 527-53-7 HCA
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)

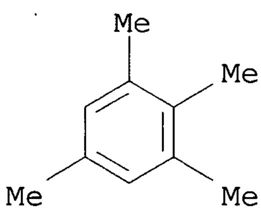


CC 35 (Noncondensed Aromatic Compounds)
IT 488-23-3, Benzene, 1,2,3,4-tetramethyl- **527-53-7**, Benzene, 1,2,3,5-tetramethyl- 1667-04-5, Mesitylene, 2-chloro-
(oxidn. by BF3-F3CCO3H)

L48 ANSWER 11 OF 12 HCA COPYRIGHT 2003 ACS
48:60246 Original Reference No. 48:10626h-i The oxidation of benzene by **hydrogen peroxide** and iron salts. Baxendale, J. H.; Magee, J. (Manchester Univ., UK). Discussions Faraday Soc., No. 14, 160-9 (Unavailable) 1953.
AB A quant. detn. of the products of the oxidation of C6H6 by Fe2+ and

H2O2 in dil. soln. has shown that PhOH and Ph2 only are formed. The variation in the amts. of these products in different conditions has led to the conclusion that the Ph radical does not react with **H2O2**, but may be reduced by ferrous ion to C6H6 and oxidized by ferric ion to PhOH. It is possible that all the PhOH is produced by the latter reaction and not by the combination of Ph and HO radicals usually assumed. In the presence of O far more oxidation of ferrous ion and C6H6 occurs than can be accounted for by the **H2O2** alone. This is explained in terms of reactions of PhOOH and PhOO radicals, the latter being produced from Ph radicals and O.

IT **527-53-7**, Benzene, 1,2,3,5-tetramethyl-
    (basicity of)
RN 527-53-7 HCA
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **7722-84-1, Hydrogen peroxide**
    (benzene oxidation by)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

CC 10 (Organic Chemistry)
IT Iron salts
    (benzene oxidation by **H2O2** in presence of)
IT 95-63-6, Benzene, 1,2,4-trimethyl- 95-93-2, Benzene, 1,2,4,5-tetramethyl- 488-23-3, Benzene, 1,2,3,4-tetramethyl- 526-73-8, Benzene, 1,2,3-trimethyl- **527-53-7**, Benzene, 1,2,3,5-tetramethyl- 700-12-9, Benzene, pentamethyl-
    (basicity of)
IT **7722-84-1, Hydrogen peroxide**
    (benzene oxidation by)

L48 ANSWER 12 OF 12 HCA COPYRIGHT 2003 ACS
39:26992 Original Reference No. 39:4335e-g Quinones. Arnold, Richard T. (Regents of the University of Minnesota). US 2373003 19450403 (Unavailable). APPLICATION: US .
AB Aromatic hydrocarbons are oxidized to their quinones with perhydrol (approx. 30% **H2O2**) in a suitable solvent at elevated temp. Thus 5 g. **durene** in 50 cc. AcOH contg. 25 cc. perhydrol is heated on a steam bath 15 hrs. The solvent is distd. and the

residue purified by steam distn. to yield 2.1 g. duroquinone, m. 110-11.degree.. From 4 g. 1-naphthaldehyde 1.1 g. 1,4-naphthoquinone, m. 124-5.degree., is obtained by diln. of the AcOH soln. with water. Similarly there are prepd. in the yields given 2-methyl-1,4-naphthoquinone, m. 104-5.degree., 30%; 2,3-dimethyl-1,4-naphthoquinone, m. 127.degree., 78%; 1,2-**benzanthraquinone** m. 166-7.degree., 46%.

CC 10 (Organic Chemistry)

=> d l49 1-8 cbib abs hitstr hitind

L49 ANSWER 1 OF 8 HCA

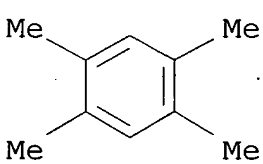
136:150735 Catalytic activation of **hydrogen peroxide** and bistrimethylsilyl peroxide for the oxidation of olefins and aromatic hydrocarbons. Kleinhenz, D.; Jost, C.; Wahl, G.; Sundermeyer, J. (Fachbereich Chemie der Philipps-Universitat Marburg, Marburg, D-35032, Germany). Selective Reactions of Metal-Activated Molecules, Proceedings of the Symposium, 3rd, Wuerzburg, Germany, Sept. 17-19, 1997, Meeting Date 1997, 57-60. Editor(s): Werner, Helmut; Schreier, Peter. Friedrich Vieweg & Sohn Verlagsgesellschaft mbH: Wiesbaden, Germany. (English) 1998. CODEN: 69BIE2.

AB Appropriate ligands can make complexes of Mo and W catalytically active in **H2O2** activation by applying a phase transfer process. On the other hand, bistrimethylsilyl peroxide is the oxidant of choice for Mo, W, and Re catalyzed oxidn. of olefins and arom. hydrocarbons in homogeneous phase.

IT **95-93-2**, 1,2,4,5-Tetramethylbenzene **7722-84-1**, **Hydrogen peroxide**, reactions
(catalytic activation of **hydrogen peroxide** and bistrimethylsilyl peroxide for the oxidn. of olefins and arom. hydrocarbons)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



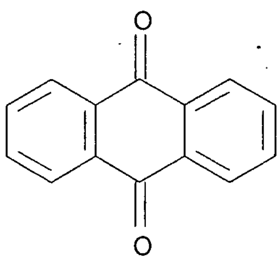
RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

IT **84-65-1P**, 9,10-Anthracenedione
(catalytic activation of **hydrogen peroxide** and bistrimethylsilyl peroxide for the oxidn. of olefins and

arom. hydrocarbons)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)
ST **hydrogen peroxide** bistrimethylsilyl peroxide
oxidn olefin arom hydrocarbon
IT Oxidation
Oxidation catalysts
(catalytic activation of **hydrogen peroxide**
and bistrimethylsilyl peroxide for the oxidn. of olefins and
arom. hydrocarbons)
IT Alkenes, reactions
Aromatic hydrocarbons, reactions
(catalytic activation of **hydrogen peroxide**
and bistrimethylsilyl peroxide for the oxidn. of olefins and
arom. hydrocarbons)
IT 70197-13-6 196614-39-8 395663-25-9 395663-26-0 395663-27-1
395663-28-2 395663-29-3 395663-30-6
(catalytic activation of **hydrogen peroxide**
and bistrimethylsilyl peroxide for the oxidn. of olefins and
arom. hydrocarbons)
IT 91-57-6, 2-Methylnaphthalene **95-93-2**, 1,2,4,5-
Tetramethylbenzene 111-66-0, 1-Octene 120-12-7, Anthracene,
reactions 142-29-0, Cyclopentene 931-88-4, Cyclooctene
5796-98-5, Bistrimethylsilyl peroxide 6443-69-2,
3,4,5-Trimethoxytoluene **7722-84-1**, **Hydrogen
peroxide**, reactions
(catalytic activation of **hydrogen peroxide**
and bistrimethylsilyl peroxide for the oxidn. of olefins and
arom. hydrocarbons)
IT 58-27-5P **84-65-1P**, 9,10-Anthracenedione 285-67-6P,
Cyclopentene oxide 286-62-4P, Cyclooctene oxide 527-17-3P,
Tetramethyl-p-**benzoquinone** 605-93-6P 605-94-7P
2984-50-1P, Hexyloxirane
(catalytic activation of **hydrogen peroxide**
and bistrimethylsilyl peroxide for the oxidn. of olefins and
arom. hydrocarbons)

L49 ANSWER 2 OF 8 HCA COPYRIGHT 2003 ACS
118:254511 Oxidation of arenes to para-**quinones** with
hydrogen peroxide catalyzed by hexafluoroacetone

hydrate. Adam, Waldemar; Ganeshpure, Pralhad A. (Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Germany). Synthesis (3), 280-2 (English) 1993. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 118:254511.

AB Various arom. hydrocarbons were oxidized with aq. **hydrogen peroxide** in the presence of hexafluoroacetone hydrate as catalyst to give p-**quinones** and/or the ring cleavage oxidn. products. The regioselective oxidn. of 2-methylnaphthalene to 2-methyl-1,4-**naphthoquinone** (vitamin K3) was studied in detail.

IT **7722-84-1**, **Hydrogen peroxide**, reactions
(oxidn. by, of arenes)

RN 7722-84-1 HCA

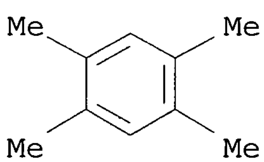
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

IT **95-93-2**
(oxidn. of, with **hydrogen peroxide**)

RN 95-93-2 HCA

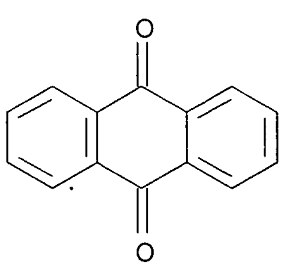
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **84-65-1P**, 9,10-Anthracenedione **106-51-4P**, 2,5-Cyclohexadiene-1,4-dione, preparation
(prepn. of)

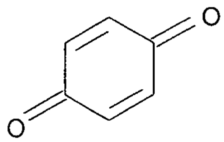
RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



RN 106-51-4 HCA

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



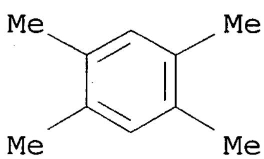
CC 25-27 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 30
ST oxidn arene; hexafluoroacetone hydrate catalyst oxidn arene; regioselective oxidn methylnaphthalene; vitamin K3; **quinone**
IT Oxidation
(of arenes with **hydrogen peroxide**, **quinones** by)
IT **7722-84-1**, **Hydrogen peroxide**, reactions
(oxidn. by, of arenes)
IT 85-01-8, Phenanthrene, reactions 91-20-3, Naphthalene, reactions 91-57-6, 2-Methylnaphthalene 93-04-9, 2-Methoxynaphthalene 95-47-6, reactions **95-93-2** 108-95-2, Phenol, reactions 120-12-7, Anthracene, reactions
(oxidn. of, with **hydrogen peroxide**)
IT 58-27-5P **84-65-1P**, 9,10-Anthracenedione **106-51-4P**, 2,5-Cyclohexadiene-1,4-dione, preparation 130-15-4P, 1,4-Naphthalenedione 434-84-4P, [9,9'-Bianthracene]-10,10'(9H,9'H)-dione 526-86-3P 527-17-3P 605-93-6P 18454-53-0P 147801-91-0P 147801-92-1P
(prepn. of)

L49 ANSWER 3 OF 8 HCA COPYRIGHT 2003 ACS
107:115120 Mechanistic studies on the oxidation of naphthalenes and methylbenzenes to **quinones** with **hydrogen peroxide** in the presence of palladium(II) catalysts. Yamaguchi, Satoru; Shinoda, Hiroyuki; Inoue, Masami; Enomoto, Saburo (Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930-01, Japan). Chemical & Pharmaceutical Bulletin, 34(11), 4467-73 (English) 1986. CODEN: CPBTAL. ISSN: 0009-2363.
AB The title oxidns. in the presence of a 0.24% Pd(II)-sulfonated polystyrene-type resin catalyst were studied. Electron-donating substituents on C-2 of naphthalenes accelerated the oxidn. A reaction path via hydroxylated intermediates was proposed. By using the MINDO/3 method, quantum chem. indexes such as the superdelocalizability for electrophilic species (SEr) and for radical species (SRr), and the net charge (Qr) of naphthalenes, methylbenzenes, and naphthols were calcd. The activity in the above reaction could be explained in terms of both Qr and SEr. The decrease of the selectivity was correlated with side reactions by radical species attacking the sites of largest SRr.
IT **7722-84-1**, **Hydrogen peroxide**, reactions
(oxidn. by, of methylbenzenes and naphthalenes with palladium catalyst, mechanism of)
RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

IT **95-93-2**, **Durene**
(oxidn. of, by **hydrogen peroxide** with
palladium catalyst, mechanism of)
RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)
ST oxidn methylbenzene naphthalene peroxide palladium; MO oxidn
methylbenzene naphthalene; **quinone** formation mechanism
IT Kinetics of oxidation
(of methylbenzenes and naphthalenes by **hydrogen
peroxide** with palladium catalyst)
IT **Quinones**
(prepn. of, from methylbenzenes and naphthalenes, mechanism of)
IT 13566-03-5, Palladium monosulfate
(catalysts, for oxidn. of methylbenzenes and naphthalenes by
hydrogen peroxide)
IT 130-15-4, 1,4-**Naphthoquinone** 524-42-5, 1,2-
Naphthoquinone
(decompn. of, by **hydrogen peroxide** in
presence of palladium catalyst)
IT **7722-84-1**, **Hydrogen peroxide**, reactions
(oxidn. by, of methylbenzenes and naphthalenes with palladium
catalyst, mechanism of)
IT 527-18-4, 2,3,5,6-**Tetramethylhydroquinone** 527-35-5,
2,3,5,6-Tetramethylphenol
(oxidn. of, by **hydrogen peroxide** with
palladium catalyst, kinetics of)
IT 91-20-3, Naphthalene, reactions 91-57-6, 2-Methylnaphthalene
91-58-7, 2-Chloronaphthalene 93-04-9, 2-Methoxynaphthalene
95-63-6, 1,2,4-Trimethylbenzene **95-93-2**, **Durene**
106-42-3, p-Xylene, reactions 581-40-8, 2,3-Dimethylnaphthalene
581-42-0, 2,6-Dimethylnaphthalene 581-89-5, 2-Nitronaphthalene
(oxidn. of, by **hydrogen peroxide** with
palladium catalyst, mechanism of)
IT 90-15-3, 1-Naphthol 7469-77-4, 2-Methyl-1-naphthol 14453-59-9,
2,3-Dimethyl-1-naphthol 110214-23-8, 2,6-Dimethyl-1-naphthol
(oxidn. of, by **hydrogen peroxide** with
palladium catalyst, selectivity of)

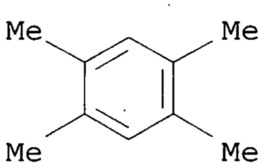
L49 ANSWER 4 OF 8 HCA COPYRIGHT 2003 ACS
106:156018 Oxidation of methylbenzenes and naphthalenes to **quinones** with **hydrogen peroxide** in the presence of a palladium catalyst. Yamaguchi, Satoru; Inoue, Masami; Enomoto, Saburo (Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930-01, Japan). Bulletin of the Chemical Society of Japan, 59(9), 2881-4 (English) 1986. CODEN: BCSJA8. ISSN: 0009-2673. OTHER SOURCES: CASREACT 106:156018.

AB Methylbenzenes and naphthalenes were oxidized to **quinones** with 60% aq. **H2O2** in acetic acid in the presence of Pd(II)-sulfonated polystyrene resin. The selectivities to **quinones** were higher in naphthalenes than in methylbenzenes. Among the naphthalenes used, 2-methylnaphthalene, 2,3-dimethylnaphthalene, and 2,6-dimethylnaphthalene, gave 1,4-**quinones** in 50-64% yields. The increase in the reaction temp. increased the selectivity to **quinones** from 40% at 20.degree. to 70% at 70.degree..

IT **95-93-2**, 1,2,4,5-Tetramethylbenzene
(regioselective oxidn. of, by **hydrogen peroxide**, polysytrene-supported palladium catalyst in)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST oxidn regiochem methylbenzene naphthalene; palladium oxidn catalyst polystyrene bound; **quinone** regiochem prepn; **naphthoquinone** regiochem prepn

IT Regiochemistry
(of oxidn. of methylbenzenes and naphthalenes to **quinones**, polystyrene supported palladium oxidn. catalysts in)

IT Oxidation catalysts
(polystyrene supported palladium, for methylbenzene and naphthalene, **quinones** by)

IT **Quinones**
(regioselective prepn. of, by oxidn. of methylbenzenes, polystyrene supported palladium oxidn. catalysts in)

IT **Quinones**
(naphtho-, regioselective prepn. of, by oxidn. of naphthalenes, polystyrene supported palladium oxidn. catalysts in)

IT 91-20-3, reactions 91-57-6, 2-Methylnaphthalene 95-63-6, 1,2,4-Trimethylbenzene **95-93-2**, 1,2,4,5-Tetramethylbenzene 106-42-3, p-Xylene, reactions 581-40-8, 2,3-Dimethylnaphthalene 581-42-0, 2,6-Dimethylnaphthalene
(regioselective oxidn. of, by **hydrogen peroxide**, polysytrene-supported palladium catalyst in)

IT 58-27-5P, 2-Methyl-1,4-naphthalenedione 130-15-4P, 1,4-**Naphthoquinone** 137-18-8P, 2,5-Dimethyl-p-**benzoquinone** 527-17-3P, Tetramethyl-p-**benzoquinone** 935-92-2P, 2,3,5-Trimethyl-p-**benzoquinone** 2197-57-1P, 2,3-Dimethyl-1,4-**naphthoquinone** 6290-94-4P, 2,6-Dimethyl-1,4-**naphthoquinone**
(regioselective prepn. of, polystyrene supported palladium oxidn. catalysts in)

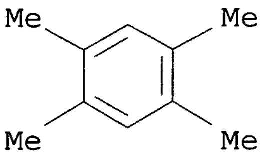
L49 ANSWER 5 OF 8 HCA COPYRIGHT 2003 ACS
96:175576 Results of toxic action of water pollutants on Daphnia magna Straus tested by an improved standardized procedure. Bringmann, Gottfried; Kuehn, Renate (Inst. Wasser-, Boden- und Lufthyg. Bundesgesundheitsamtes, Berlin, 1000/33, Fed. Rep. Ger.). Zeitschrift fuer Wasser- und Abwasser-Forschung, 15(1), 1-6 (German) 1982. CODEN: ZWABAQ. ISSN: 0044-3727.

AB A largely standardized procedure for testing the potential toxic action of water pollutants involves measuring the immobilization of D. magna. The standardized test strain IRCHA was used. The stock cultures were fed standardized dry algae. Testing of the toxic action of the water pollutants was performed in a chem. and phys. defined standardized culture medium (artificial fresh water). When evaluating the test results, the mean effective concn. (EC50) values of the substances tested were detd. according to a math. standardized method. The toxicol. relevant range of the EC was detd. by establishing the EC0 and the EC100. The results for 183 pollutants are tabulated by compd. classes. EC50 values <10 mg/L were detected. In the group of the toxicol. effective cations tested, the EC50 was: Ag <0.01, Hg and Cu <0.1, and Tl and Cd <1 mg/L. In the group of the toxicol. effective anions tested, the EC50 was: chromate <1, cyanide, iodide, and selenate <10, and sulfide and arsenate 10 mg/L. Other toxicol. effective inorg. substances, such as **H2O2** (30%) and N2H5OH (80%), had an EC50 <10 mg/L. In the groups of the org. substances tested, the EC50 for **hydroquinone** [**123-31-9**], 4-nonylphenol [104-40-5], and pentachlorophenol [87-86-5] was <1 mg/L, and <10 mg/L for salicylaldehyde [90-02-8], cumene hydroperoxide [80-15-9], 2,4-dinitrophenol [51-28-5], 4,6-dinitro-o-cresol [534-52-1], 4-nitro-m-cresol [2581-34-2], 4-nitrotoluene [99-99-0], 2,3-dinitrotoluene [602-01-7], .alpha.-chlorotoluene [100-44-7], 2,4-dichlorophenol [120-83-2], 3,5-dichlorophenol [591-35-5], 2,4,5-trichlorophenol [95-95-4], p-chloroaniline [106-47-8], and Na dodecylbenzenesulfonate [25155-30-0].

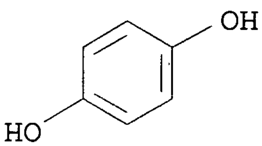
IT **95-93-2 123-31-9**, biological studies
7722-84-1, biological studies
(toxicity of, to Daphnia magna, by improved standardized procedure)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 123-31-9 HCA
CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO— OH

CC 4-3 (Toxicology)
IT 50-00-0, biological studies 51-28-5, biological studies 56-23-5, biological studies 56-81-5, biological studies 57-12-5, biological studies 57-13-6, biological studies 60-00-4, biological studies 60-29-7, biological studies 60-35-5, biological studies 62-53-3, biological studies 64-17-5, biological studies 64-19-7, biological studies 65-85-0, biological studies 67-56-1, biological studies 67-63-0, biological studies 67-64-1, biological studies 69-72-7, biological studies 71-23-8, biological studies 71-36-3, biological studies 71-41-0, biological studies 71-43-2, biological studies 71-55-6 75-04-7, biological studies 75-05-8, biological studies 75-09-2, biological studies 75-85-4 75-87-6 76-03-9, biological studies 77-92-9, biological studies 78-40-0 78-83-1, biological studies 78-92-2 78-93-3, biological studies 79-01-6, biological studies 79-10-7, biological studies 80-15-9 80-62-6 84-66-2 87-86-5 88-72-2 88-75-5 88-89-1 90-02-8, biological studies 95-48-7, biological studies 95-49-8 95-50-1 95-53-4, biological studies 95-68-1 **95-93-2** 95-95-4 96-41-3 98-00-0 98-01-1, biological studies 98-06-6 98-07-7 98-82-8 98-95-3, biological studies 99-08-1 99-65-0 99-99-0 100-01-6, biological studies 100-02-7, biological studies 100-41-4, biological studies 100-42-5, biological studies 100-44-7, biological studies 100-47-0, biological studies 100-51-6, biological studies 102-71-6, biological studies 103-11-7 104-40-5 105-37-3 105-54-4 105-60-2, biological studies 106-47-8, biological studies 106-89-8, biological studies

107-06-2, biological studies 107-11-9 107-15-3, biological studies 107-19-7 107-21-1, biological studies 107-88-0 107-92-6, biological studies 108-05-4, biological studies 108-10-1 108-21-4 108-24-7 108-31-6, biological studies 108-39-4, biological studies 108-88-3, biological studies 108-90-7, biological studies 108-91-8, biological studies 108-94-1, biological studies 108-95-2, biological studies 109-57-9 109-60-4 109-99-9, biological studies 110-12-3 110-16-7, biological studies 110-19-0 110-54-3, biological studies 110-82-7, biological studies 110-83-8, biological studies 110-86-1, biological studies 110-91-8, biological studies 111-27-3, biological studies 111-42-2, biological studies 111-46-6, biological studies 111-55-7 111-69-3 111-70-6 111-87-5, biological studies 112-27-6 112-30-1 112-34-5 115-77-5, biological studies 118-96-7 119-33-5 120-82-1 120-83-2 120-92-3 121-14-2 122-79-2 **123-31-9**, biological studies 123-42-2 123-54-6, biological studies 123-72-8 123-86-4 123-91-1, biological studies 126-73-8, biological studies 127-18-4, biological studies 131-17-9 139-13-9 141-32-2 141-43-5, biological studies 141-78-6, biological studies 141-97-9 142-96-1 144-49-0 150-76-5 151-21-3, biological studies 151-56-4, biological studies 291-64-5 463-57-0 534-22-5 534-52-1 540-88-5 554-12-1 554-84-7 583-60-8 591-35-5 602-01-7 606-20-2 622-45-7 623-37-0 626-93-7 628-63-7 628-92-2 700-38-9 1330-20-7, biological studies 1330-43-4 2581-34-2 3811-04-9 7439-97-6, biological studies 7440-02-0, biological studies 7440-22-4, biological studies 7440-28-0, biological studies 7440-36-0, biological studies 7440-38-2, biological studies 7440-42-8, biological studies 7440-43-9, biological studies 7440-47-3, biological studies 7440-50-8, biological studies **7722-84-1**, biological studies 7778-43-0 7778-74-7 7782-49-2, biological studies 10102-18-8 10588-01-9 12208-13-8 14797-65-0, biological studies 18496-25-8 20461-54-5, biological studies 24552-04-3 24959-67-9, biological studies 25155-30-0 26952-21-6 65492-74-2
(toxicity of, to Daphnia magna, by improved standardized procedure)

L49 ANSWER 6 OF 8 HCA

66:2042 Direct oxidation of **durene** to a cyclohexadienone. Chemistry and photolysis. Hart, Harold; Lange, Richard M. (Michigan State Univ., East Lansing, MI, USA). Journal of Organic Chemistry, 31(11), 3776-9 (English) 1966. CODEN: JOCEAH. ISSN: 0022-3263.

GI For diagram(s), see printed CA Issue.

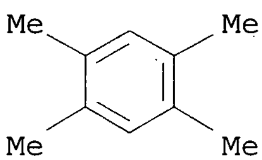
AB The major oxidn. product of **durene** with F3CCO2OH-BF3 in CH2Cl2, or with 90% **H2O2** in AcOH-H2SO4 was 3,4,6,6-tetramethyl-2,4-cyclohexadienone (I), which could be obtained in yields >75%. **Duroquinone**, **durohydroquinone**, and durophenol were among the minor oxidn. products. The dienone gave a Diels-Alder adduct with maleic anhydride, and was readily converted to the cross-conjugated

6-methylene-1,4-cyclohexadienes (II and III) by 1,2 addn. of methyl Grignard, or redn. with LiAlH4, followed by 1,4 dehydration of the resulting als. I was recovered from prolonged irradiation (Pyrex) in moist or anhyd. ether, but in EtOH it was rapidly photolyzed with ring opening to give Et 3,4,6-trimethylhepta-3,5-dienoate in an excellent yield. The presence or absence of certain Me groups in 2,4-cyclohexadienones can completely alter their photochem. behavior.

IT **95-93-2**
(oxidn. of)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



CC 22 (Physical Organic Chemistry)

ST CYCLOHEXADIENONES OXIDN **DURENE**; OXIDN **DURENE** CYCLOHEXADIENONES; PHOTOLYSIS CYCLOHEXADIENONES; **DURENE** CYCLOHEXADIENONES OXIDN

IT **95-93-2**
(oxidn. of)

L49 ANSWER 7 OF 8 HCA COPYRIGHT 2003 ACS

54:128656 Original Reference No. 54:24562c-i,24563a-e Reductions in liquid ammonia. XIII. Reduction and reductive methylation of 2-methyl- and 1,2,3-trimethylnaphthalene; isopropylation of naphthalene. Huckel, Walter; Cramer, Rolf; Laufer, Siegmar (Univ. Tubingen, Germany). Ann., 630, 89-104 (Unavailable) 1960.

AB cf. CA 53, 6167e. Redn. of 2-C10H7Me (I) with Na and EtOH (Method A) or with Na and NH3 (Method B) (CA 34, 962) gave a mixt. of largely 3,4-dihydro-2-methylnaphthalene (II) and some 1,4-dihydro-2-methylnaphthalene (III), while Birch redn. (Method C) gave only III. Birch redn. with much excess Na gave 1,4,5,8-tetrahydro-2-methylnaphthalene (IV). All dihydronaphthalenes were oxidized with HNO3 to phthalic acid. III and analogs gave solid adducts with Hg(OAc)2 (V) while II did not; IV added 2 moles V. II and analogs had more intense ultraviolet absorption and greater exaltation of the mol. refraction (EMRD) than III. MeBr added to the redn. of I by Method B gave a dihydro-1,2,3-trimethylnaphthalene (VI) isomeric with that (VIa) obtained by redn. of 1,2,3-C10H5Me3 (VII). VI and VIa were the 2 possible dihydro derivs. with the double bond in the methylated ring conjugated with the unmethylated benzene ring, or possibly different mixts. of these; infrared absorption favored 3,4-dihydro-1,2,3-trimethylnaphthalene being or predominating in VI. Method A. I (30 g.) in 500 cc. warm EtOH was reduced with 35 g. Na and the distd. product in 50 cc. ether shaken with 67.5 g. V in 450 cc. H2O to give

27.8 g. V adduct of III, m. 146.degree.; this with 25% HCl gave 9.5 g. III, b13 106-7.degree., d20 0.9785, nD20 1.5527, EMRD +0.34, .lambda.max. (log .epsilon.) 270 (2.92), 280 m.mu. (2.89), .lambda.min. (log .epsilon.) 273 m.mu. (2.60); the filtrate from the V adduct gave 14.7 g. I picrate, m. 115.degree., and after chromatography 15.0 g. II, b13 105.degree., d20 0.9743, nD20 1.5720, EMRD +1.97, .lambda.max. (log .epsilon.) 268 m.mu. (3.82) [dibromide (prepd. in MeOH at -70.degree.) m. 34.degree.]. II ozonized in MeOH at -15.degree. and the ozonide decompd. with alk. **H2O2** gave an acid, C11H12O3, m. 105.degree., presumably o-(3-oxobutyl)benzoic acid. Method B. Addn. of 21.45 g. I in 150 cc. ether to 6.9 g. Na in 200 cc. NH3 at -75.degree. and decompn. of the deep red mixt. with 18 g. NH4Cl after 50 min. stirring under N gave 86% II, 8.5% III, and 6.5% recovered I, possibly formed from II during the treatment with V. A similar expt., in which 6.9 g. addnl. Na and 200 cc. NH3 was added after the NH4Cl treatment and another 18 g. NH4Cl 30 min. later gave 19 g. 1,2,3,4-tetrahydro-2-methylnaphthalene (VIII), b14 98.degree., d20 0.9591, nD20 1.5370, EMRD +0.41, .lambda.max. (log .epsilon.) 268 (3.27), 273 m.mu. (3.26), unchanged by cold Br or KMnO4. Redn. of II by Method B also gave VIII. Method C. Na (4.7 g.) was added to 10.0 g. I, 12.5 g. MeOH, 50 cc. ether, and 300 cc. NH3 at -60.degree. and the blue color disappeared after 90 min.; this furnished 60% III, 35% I, no evidence of II or IV. In a similar expt., 0.5 g. reduced Cu was added before the Na and this gave 28% III and 40% I. An expt. with 10 g. I, 15 g. Na, 50 cc. ether, 40 cc. MeOH, and 400 cc. NH3 required 4 hrs. to discharge the blue color and yielded 7 g. IV, m. 21.degree., d25 0.9591, nD25 1.5276, EMRD -0.28, .lambda.max. (log .epsilon.) 255 m.mu. (2.71); adduct with 2 moles V m. 128.degree., unchanged by 20% NaOEt at 100.degree. or by further redn. by Methods A or C. IV (3 g.) and 1 g. Raney Ni in EtOH under N gave a mixt. of I and VIII. VII (17.0 g.) reduced by Method B 4 hrs. gave 14.5 g. VI, b17 113-16.degree., d20 0.9792, nD25 1.5818, EMRD +2.73, .lambda.max. (log .epsilon.) 255 m.mu. (4.59), unreactive with V and giving an oily dibromide. MeBr (19.0 g.) condensed in the red soln. of 14.2 g. I, 4.6 g. Na, 100 cc. ether, and 200 cc. NH3 below -33.degree., the resulting colorless soln. freed of NH3, and extd. with ether gave 12.0 g. VIa, b64 142-9.degree., m. 4-5.degree., d20 0.9704, nD20 1.5861, EMRD +2.12, .lambda.max. (log .epsilon.) 258 m.mu. (4.40), unreactive with V and giving an oily dibromide. VIa (8.5 g.) and 7.5 g. **quinone** in 35 cc. dioxane heated 24 hrs. at 130.degree. under N, dild. with petr. ether to ppt. **hydroquinone**, and the filtrate chromatographed on active Al2O3 gave VII, m. 28.4.degree.; picrate m. 141.degree., .lambda.max. (log .epsilon.) 268 (3.95), 275 m.mu. (3.97). In PhOMe this reaction was unsuccessful. VIa was also dehydrogenated to VII in 92% yield over asbestos contg. 30% Pd 24 hrs. at 240-60.degree.. The crude VIa (from 28.4 g. I) with 6.94 g. addnl. Na and 28.68 g. MeBr in 150 cc. ether and 200 cc. NH3 gave 23 g. 1,2,3,4-tetrahydro-1,2,3,4-tetramethylnaphthalene, b12 133-6.degree., d20 0.9426, nD20 1.5321, EMRD -0.78, .lambda.max. (log .epsilon.) 265 (2.787), 273 m.mu. (2.772), dehydrogenated to

1,2,3,4-C10H4Me4, m. 47.degree., .lambda.max. (log .epsilon.) 290 m.mu. (3.94). Reductive alkylation of 17 g. VII with 4.6 g. Na, 18.9 g. MeBr, 250 cc. NH3, and 100 cc. ether gave a 1,2-dihydropentamethylnaphthalene with all Me groups in the reduced ring, b11 106-10.degree., d20 0.9752, nD20 1.5759, EMRD +2.76, .lambda.max. (log .epsilon.) 266 m.mu. (4.01). Me2CHBr (IX) (49.2 g.) stirred 2 hrs. at -60 to -40.degree. with the red soln. of 9.2 g. Na, 25.5 g. C10H8, 300 cc. NH3, and 150 cc. ether, the NH3-free residue extd. with ether, and distd. gave 23 g. 1,4-dihydro-1,4-diisopropylnaphthalene (X), b12, 155-9.degree., d20 0.9451, nD20 1.5302, EMRD +0.25, .lambda.max. (log .epsilon.) 265 m.mu. (3.58); dibromide m. 69.degree., did not add V. Dehydrogenation of X by **quinone** in dioxane or with Pd catalyst 5 hrs. at 280-300.degree. gave 66-70% 1,4-C10H6(CHMe2)2 (XI), b735 272-4.degree., b12 157-61.degree., d20 1.0073, nD20 1.5783, also prepd. from 1,4-C10H6Br2 (Bayer and O'Reilly, CA 52, 16308f), Na, and IX. Boiling 5 g. XI with 5% HNO3 7 days gave 0.3 g. 1,4-C10H6(CO2H)2, m. 322.degree.; di-Me ester m. 64.degree.. Catalytic dehydrogenation of X 50 hrs. and oxidn. of the product with 5% HNO3 gave 1-C10H7CO2H. Birch redn. of **durene** (XII) failed owing to insoly. in the reaction mixt., but succeeded when a precooled soln. of 2.5 g. XII in 50 cc. PhMe and 50 cc. MeOH was added to 400 cc. NH3 contg. 50 g. Na at -60.degree.; the opalescent mixt. was warmed to -35.degree., decolorized with MeOH, and the resulting hydrocarbon mixt. reduced twice more. After removal of dihydrotoluene by fractional distn., crystn. of the residue from 10 cc. ether at -70.degree. gave 0.2 g. 3,6-dihydrodurene, m. 61.9-2.2.degree., transparent above .lambda. 250 m.mu., analyzed by hydrogenation and BzO2H titration.

CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)

L49 ANSWER 8 OF 8 HCA

34:33549 Original Reference No. 34:5075c-d **Quinones** by the peroxide oxidation of aromatic compounds. Arnold, Richard T.; Larson, Raymond J. Org. Chem., 5, 250-2 (Unavailable) 1940. CODEN: JOCEAH. ISSN: 0022-3263.

AB 1-Naphthaldehyde, naphthalene, **durene**, o-xylene, 2-methylnaphthalene, 2,3-dimethylnaphthalene, 1,2-benzanthracene and pyrene (I) on oxidation with 30% **H2O2** in glacial AcOH give the corresponding **quinones** in yields similar to those obtained by Cr2O3 oxidation. In the case of I, a mixt. of 3,8- and 3,10-**pyrenequinones** is obtained which could not be sepd. The greatest value of the reaction lies in the selective oxidation of alkyl polycyclic derivs.

CC 10 (Organic Chemistry)

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L1                1 SEA "HYDROGEN PEROXIDE"/CN
                    E ISODURENE/CN
L2                1 SEA ISODURENE/CN
                    E C10H14/MF
L3             1272 SEA C10H14/MF
L4             1187 SEA ?TETRAMETHYLBENZEN?/CNS
L5               17 SEA L3 AND L4

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                    E TETRAHYDRO ANTHRAQUINONE/CN

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L9              324 SEA 2508.17.36/RID
L10           62656 SEA 2508.17.45/RID
L11            1336 SEA L10 AND ?TETRAHYDRO?/CNS
L12             579 SEA L11 AND 3/ELC.SUB
L13              34 SEA L12 AND IDS/CI
L14           61320 SEA L10 NOT L11
L15            9709 SEA L14 AND 3/ELC.SUB
L16            1219 SEA L15 AND 2/O
L17           23256 SEA ANTHRACENEDIONE#
L18             336 SEA L16 AND L17
L19           20548 SEA L14 AND L17
                    E ANTHRAQUINONE/CN
L20               1 SEA ANTHRAQUINONE/CN
                    E DURENE/CN
L21               1 SEA DURENE/CN
L22               1 SEA L21 AND L5
                    E QUINONE/CN
L23               1 SEA QUINONE/CN
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                E HYDROQUINONE/CN
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                TETRAHYDRO#(2A)ANTHRAQUINONE#
L26       33147 SEA L20 OR L18 OR ANTHRAQUINONE#
L27       84976 SEA L23 OR QUINONE# OR L24 OR HYDROQUINONE#
L28        1077 SEA L2 OR ISODURENE#

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L31        3637 SEA (L25 OR L26) AND L27
L32           4 SEA L31 AND L28
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L34          16 SEA L33 NOT L32

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                OR MADE# OR MAKING# OR FABRICAT? OR SYNTHESI? OR PREPAR?
                OR PREP#)(2A)(HYDROGEN#(A)PEROXIDE# OR H2O2)
L37           1 SEA L36 AND L28
L38           2 SEA L36 AND L30
L39      163261 SEA L1 OR HYDROGEN#(A)PEROXIDE# OR H2O2
L40           7 SEA L39 AND L28
L41           1 SEA L40 AND (L25 OR L26 OR L27)
L42          38 SEA L39 AND L30
L43          12 SEA L42 AND (L25 OR L26 OR L27)
L44       40941 SEA ?ANTHRAQUINON?
L45           5 SEA L39 AND (L28 OR L30) AND L44
L46      174042 SEA ?QUINON?
L47          14 SEA L39 AND (L28 OR L30) AND L46
L48          12 SEA L37 OR L38 OR L40 OR L41 OR L45
L49           8 SEA (L43 OR L47) NOT L48

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L32 ANSWER 1 OF 4 HCA COPYRIGHT 2003 ACS

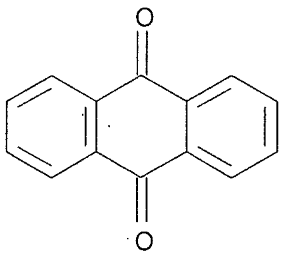
137:262700 Hydrocarbon Oxidation by Bis-.mu.-oxo Manganese Dimers: Electron Transfer, Hydride Transfer, and Hydrogen Atom Transfer Mechanisms. Larsen, Anna S.; Wang, Kun; Lockwood, Mark A.; Rice, Gordon L.; Won, Tae-Jin; Lovell, Scott; Sadilek, Martin; Turecek, Frantisek; Mayer, James M. (Department of Chemistry, University of Washington, Seattle, WA, 98195-1700, USA). Journal of the American Chemical Society, 124(34), 10112-10123 (English) 2002. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB Described here are oxidns. of alkylarom. compds. by dimanganese .mu.-oxo and .mu.-hydroxo dimers [(phen)2MnIV(.mu.-O)2MnIV(phen)2]4+ ([Mn2(O)2]4+), [(phen)2MnIV(.mu.-O)2MnIII(phen)2]3+ ([Mn2(O)2]3+), and [(phen)2MnIII(.mu.-O)(.mu.hydroxyl)MnIII(phen)2]3+ ([Mn2(O)(OH)]3+). Dihydroanthracene, xanthene, and fluorene are oxidized by [Mn2(O)2]3+ to give anthracene, bixanthenyl, and bifluorenyl, resp. The Mn product is the bis(hydroxide) dimer, [(phen)2MnIII(.mu.hydroxyl)2MnII(phen)2]3+ ([Mn2(OH)2]3+). Global anal. of the UV/visible spectral kinetic data shows a consecutive reaction with buildup and decay of [Mn2(O)(OH)]3+ as an intermediate. The kinetics and products indicate a mechanism of H atom transfers from the substrates to oxo groups of [Mn2(O)2]3+ and [Mn2(O)(OH)]3+. [Mn2(O)2]4+ is a much stronger oxidant, converting toluene to tolyl-phenylmethanes and naphthalene to binaphthyl. Kinetic and mechanistic data indicate a mechanism of initial preequil. electron transfer for p-methoxytoluene and naphthalenes because, for instance, the reactions are inhibited by addn. of [Mn2(O)2]3+. The oxidn. of toluene by [Mn2(O)2]4+, however, is not inhibited by [Mn2(O)2]3+. Oxidn. of a mixt. of C6H5CH3 and C6H5CD3 shows a kinetic isotope effect of 4.3 .+-. 0.8, consistent with C-H bond cleavage in the rate-detg. step. The data indicate a mechanism of initial hydride transfer from toluene to [Mn2(O)2]4+. Thus, oxidns. by Mn oxo dimers occur by three different mechanisms: H atom transfer, electron transfer, and hydride transfer. The thermodn. of e-, H.bul., and H- transfers were detd. from redox potential and pKa measurements. For a particular oxidant and a particular substrate, the choice of mechanism is influenced both by the thermochem. and by the intrinsic barriers. Rate consts. for H atom abstraction by [Mn2(O)2]3+ and [Mn2(O)(OH)]3+ are consistent with their 79 and 75 kcal mol-1 affinities for H.bul.. In the oxidn. of p-methoxytoluene by [Mn2(O)2]4+, hydride transfer is thermochem. 24 kcal mol-1 more facile than electron transfer; yet the latter mechanism is preferred. Thus, electron transfer has a substantially smaller intrinsic barrier than does hydride transfer in this system.

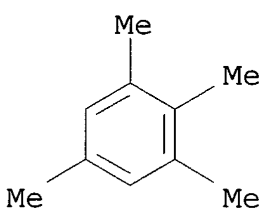
IT **84-65-1P**, 9,10-**Anthraquinone**
(electron transfer, hydride transfer, and hydrogen atom transfer mechanisms in hydrocarbon oxidn. by bis-.mu.-oxo manganese dimers)

RN 84-65-1 HCA

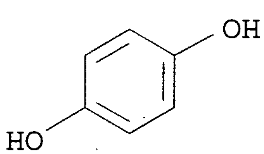
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



IT 527-53-7, 1,2,3,5-Tetramethylbenzene
(electron transfer, hydride transfer, and hydrogen atom transfer mechanisms in hydrocarbon oxidn. by bis-.mu.-oxo manganese dimers)
RN 527-53-7 HCA
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **123-31-9**, **Hydroquinone**, reactions
(in conversion to .mu.-oxo manganese dimer; electron transfer, hydride transfer, and hydrogen atom transfer mechanisms in hydrocarbon oxidn. by bis-.mu.-oxo manganese dimers)
RN 123-31-9 HCA
CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 67, 72, 75
IT **84-65-1P**, 9,10-**Anthraquinone** 90-44-8P, Anthrone
1530-12-7P, Bifluorenyl 1940-57-4P, 9-Bromofluorene 42343-24-8P
53039-57-9P 69180-12-7P 463962-43-8P
(electron transfer, hydride transfer, and hydrogen atom transfer mechanisms in hydrocarbon oxidn. by bis-.mu.-oxo manganese dimers)
IT 86-73-7, Fluorene 90-12-0, 1-Methylnaphthalene 91-20-3, Naphthalene, reactions 91-57-6, 2-Methylnaphthalene 92-83-1, Xanthene 95-93-2, Durene 104-93-8, p-Methoxytoluene 106-42-3,

p-Xylene, reactions 108-38-3, m-Xylene, reactions 108-88-3, Toluene, reactions **527-53-7**, 1,2,3,5-Tetramethylbenzene 573-98-8, 1,2-Dimethylnaphthalene 613-31-0, 9,10-Dihydroanthracene 1124-18-1
(electron transfer, hydride transfer, and hydrogen atom transfer mechanisms in hydrocarbon oxidn. by bis-.mu.-oxo manganese dimers)

IT **123-31-9**, **Hydroquinone**, reactions
(in conversion to .mu.-oxo manganese dimer; electron transfer, hydride transfer, and hydrogen atom transfer mechanisms in hydrocarbon oxidn. by bis-.mu.-oxo manganese dimers)

L32 ANSWER 2 OF 4 HCA COPYRIGHT 2003 ACS

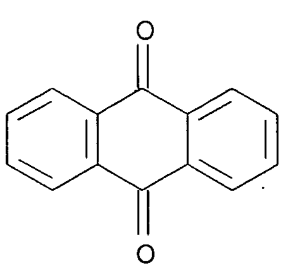
136:56010 Process for manufacture of hydrogen peroxide and composition for use therein. Nystroem, Mats; Jaernvik, Christina (Akzo Nobel N.V., Neth.; Eka Chemicals AB). PCT Int. Appl. WO 2001098204 A1 20011227, 10 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-SE1192 20010528. PRIORITY: EP 2000-850109 20000619; US 2000-PV212633 20000619.

AB The invention relates to a process for prodn. of hydrogen peroxide according to the **anthraquinone** process including alternate hydrogenation and oxidn. of one or more **quinones** selected from **anthraquinones** and/or **tetrahydro anthraquinones** in a working soln. comprising at least one **quinone** solvent and at least one **hydroquinone** solvent, wherein said at least one **quinone** solvent comprises **isodurene** in an amt. from 15 wt.% to 100 wt%. The invention also relates to a compn. useful as a working soln. at prodn. of hydrogen peroxide.

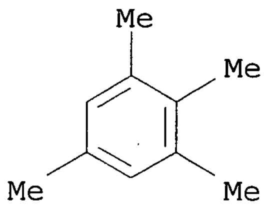
IT **84-65-1**, 9,10-Anthracenedione **527-53-7** **28758-94-3**
(process for manuf. of hydrogen peroxide and compn. for use therein)

RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



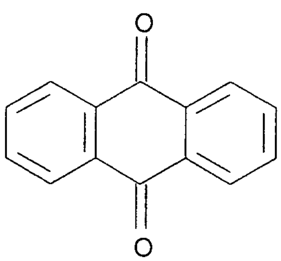
RN 527-53-7 HCA
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 28758-94-3 HCA
CN 9,10-Anthracenedione, tetrahydro- (9CI) (CA INDEX NAME)

CM 1

CRN 84-65-1
CMF C14 H8 O2



IC ICM C01B015-023
CC 49-8 (Industrial Inorganic Chemicals)
ST hydrogen peroxide manuf **anthraquinone** process
IT **Quinones**
(process for manuf. of hydrogen peroxide and compn. for use therein)
IT **84-65-1**, 9,10-Anthracenedione 108-82-7 **527-53-7**
4559-86-8 **28758-94-3**
(process for manuf. of hydrogen peroxide and compn. for use therein)

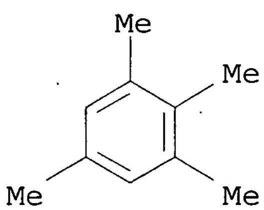
L32 ANSWER 3 OF 4 HCA
110:153841 Mediated electrochemical synthesis of aromatic aldehydes, ketones, and **quinones** using ceric methanesulfonate. Kreh, Robert P.; Spotnitz, Robert M.; Lundquist, Joseph T. (Washington Res. Cent., W. R. Grace and Co., Columbia, MD, 21044, USA). Journal of Organic Chemistry, 54(7), 1526-31 (English) 1989. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 110:153841.
AB Cerium (IV) in aq. methanesulfonic acid is an excellent reagent for the oxidn of alkyl aroms. and polycyclic aroms. to aldehydes, ketones, and **quinones**. The benefits of methanesulfonic

acid include low cost, low nucleophilicity, stability to anodic, and electrochem. oxidn. and high soly. of Ce(III) and Ce(IV) in aq. solns. of this acid. The properties of this medium are ideal for electrochem. regeneration, giving current efficiencies up to 89% at 500 mA/cm2. With this system, enhanced yields of menadione were obtained by adding Cr(VI). A new solid oxidant, Ce(CH3SO3)2(OH)2.cntdot.H2O, was produced electrochem., providing a convenient starting material for these oxidns. Improved selectivity was obtained in the synthesis of m-phenoxybenzaldehyde by using this solid material in place of sol. Ce(IV).

IT **527-53-7**, 1,2,3,5-Tetramethylbenzene
(electrochem. oxidn. of, with ceric methanesulfonate)

RN 527-53-7 HCA

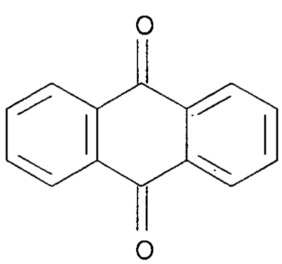
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **84-65-1P**, 9,10-**Anthraquinone**
(prepn. of, from electrochem. oxidn. of anthracene)

RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST carbonyl compd aryl electrochem synthesis; ceric methanesulfonate electrochem oxidn; ketone aryl electrochem synthesis; aldehyde aryl electrochem synthesis; **quinone** aryl electrochem synthesis

IT Aldehydes, preparation
Ketones, preparation
Quinones
(aryl, prepn. of, from electrochem. oxidn. of alkyl and polycyclic arom. compds.)

IT 86-57-7, 1-Nitronaphthalene 91-20-3, Naphthalene, reactions 91-57-6, 2-Methylnaphthalene 95-47-6, reactions 95-49-8, o-Chlorotoluene 98-51-1, p-tert-Butyltoluene 99-87-6, p-Isopropyltoluene 100-41-4, Ethylbenzene, reactions 100-42-5,

reactions 106-42-3, p-Xylene, reactions 106-43-4, p-Chlorotoluene 108-38-3, reactions 108-88-3, reactions 119-64-2, 1,2,3,4-Tetrahydronaphthalene 120-12-7, Anthracene, reactions **527-53-7**, 1,2,3,5-Tetramethylbenzene 622-96-8, p-Ethyltoluene 2876-35-9, 2-tert-Butylnaphthalene
(electrochem. oxidn. of, with ceric methanesulfonate)

IT **84-65-1P**, 9,10-**Anthraquinone**
(prepn. of, from electrochem. oxidn. of anthracene)

L32 ANSWER 4 OF 4 HCA COPYRIGHT 2003 ACS

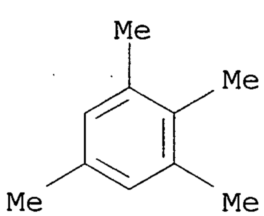
106:127956 Electrochemical oxidation of aromatic compounds using ceric ions in aqueous methanesulfonic acid. Kreh, Robert P.; Spotnitz, Robert M. (Grace, W. R., and Co., USA). U.S. US 4639298 A 19870127, 7 pp. (English). CODEN: USXXAM. APPLICATION: US 1986-859548 19860505.

AB **Quinones** and arom. aldehydes or ketones are formed from the corresponding arom. and alkyl arom. compds. in good yields and selectivity by an indirect electrochem. oxidn. process involving ceric methanesulfonate. An in-cell oxidn. was done by mixing 20 mL p-tert-butyltoluene with 200 mL of a soln. of 4.6M methanesulfonic acid and 0.8M Ce(III) methanesulfonate. The mixt., used as an anolyte, was heated to 60.degree. at a current of 110 mA/cm2 in an electrochem. cell contg. a Pt anode, steel cathode, and Nafion ion-exchange membrane until 0.15 Faraday charge was passed. Anal. of the anolyte revealed that p-tert-benzaldehyde was produced with a current efficiency of 68%, and a selectivity based on p-tert-butyltoluene of 83%.

IT **527-53-7**, 1,2,3,5-Tetramethylbenzene
(oxidn. of, electrochem., ceric ions in)

RN 527-53-7 HCA

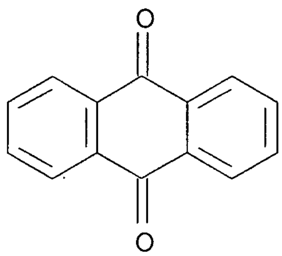
CN Benzene, 1,2,3,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **84-65-1P, Anthraquinone**
(prepn. of, electrochem., ceric ions in)

RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



IC ICM C25B003-02
NCL 204-59R
CC 72-9 (Electrochemistry)
Section cross-reference(s): 25, 43, 62, 63
IT 86-57-7, 1-Nitronaphthalene 91-20-3, reactions 91-57-6, 2-Methylnaphthalene 95-47-6, reactions 95-49-8, o-Chlorotoluene 98-51-1, p-tert-Butyltoluene 99-87-6, p-Isopropyltoluene 100-41-4, Ethyl benzene, reactions 100-42-5, reactions 104-93-8, p-Methylanisole 106-42-3, reactions 106-43-4, p-Chlorotoluene 108-38-3, reactions 108-41-8, m-Chlorotoluene 108-88-3, reactions 120-12-7, Anthracene, reactions **527-53-7**, 1,2,3,5-Tetramethylbenzene 622-96-8, p-Ethyltoluene 1009-01-4, o-Tolyl methanesulfonate 62690-59-9, 1,2,3,5-Tetrahydronaphthalene
(oxidn. of, electrochem., ceric ions in)
IT 58-27-5P, 2-Methyl-1,4-naphthoquinone **84-65-1P**, **Anthraquinone** 89-98-5P, o-Chlorobenzaldehyde 98-86-2P, Acetophenone, preparation 100-52-7P, Benzaldehyde, preparation 104-87-0P, p-Tolualdehyde 104-88-1P, p-Chlorobenzaldehyde, preparation 122-00-9P, p-Methylacetophenone 122-03-2P, p-Isopropylbenzaldehyde 123-11-5P, p-Anisaldehyde, preparation 130-15-4P, 1,4-Naphthoquinone 487-68-3P, 2,4,6-Trimethylbenzaldehyde 529-20-4P, o-Tolualdehyde 529-34-0P, 1-Tetralone 587-04-2P, m-Chlorobenzaldehyde 605-93-6P, 6-Methyl-1,4-naphthoquinone 620-23-5P, m-Tolualdehyde 939-97-9P, p-tert-Butylbenzaldehyde 4748-78-1P, p-Ethylbenzaldehyde 17788-47-5P, 5-Nitro-1,4-naphthoquinone 107331-38-4P, o-Salicyl methanesulfonate
(prepn. of, electrochem., ceric ions in)

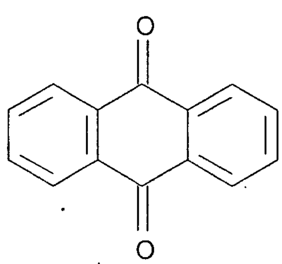
=> d l34 1-16 cbib abs hitstr hitind

L34 ANSWER 1 OF 16 HCA COPYRIGHT 2003 ACS
131:314140 The correlation and prediction of the solubility of compounds in water using an amended solvation energy relationship. Abraham, Michael H.; Le, Joelle (Department of Chemistry, University College London, London, WC1H OAJ, UK). Journal of Pharmaceutical Sciences, 88(9), 868-880 (English) 1999. CODEN: JPMSAE. ISSN: 0022-3549. Publisher: American Chemical Society.
AB The aq. soly. of liqs. and solids, as log SW, has been correlated with an amended solvation equation that incorporates a term in

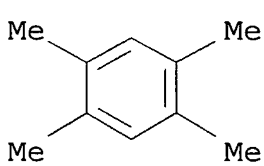
.SIGMA..alpha.2H .times. .SIGMA..beta.2H, where the latter are the hydrogen bond acidity and basicity of the solutes, resp. Application to a training set of 594 compds. led to a correlation equation with a std. deviation, SD, of 0.56 log units. For a test set of 65 compds., the SD was 0.50 log units, and for a combined correlation equation for 659 compds., the SD was 0.56 log units. The correlation equations enable the factors that influence aq. soly. to be revealed. The hydrogen-bond propensity of a compd. always leads to an increase in soly., even though the .SIGMA..alpha.2H .times. .SIGMA..beta.2H term opposes soly. due to interactions in the liq. or solid. Increase in solute dipolarity/polarizability increases soly., whereas an increase in solute excess molar refraction, and esp., vol. decrease soly. The soly. of Bronsted acids and bases is discussed, and corrections for the fraction of neutral species in the satd. soln. are graphically presented.

IT **84-65-1**, **Anthraquinone 95-93-2**, 1,2,4,5-Tetramethylbenzene **123-31-9**, 1,4-Benzenediol, properties
(correlation and prediction of the soly. of compds. in water using an amended solvation energy relationship)

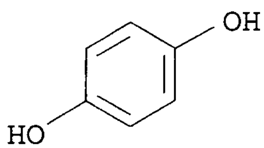
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 123-31-9 HCA
CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 22
IT 50-02-2, Dexamethasone 50-03-3, Hydrocortisone 21-acetate 50-06-6, Phenobarbital, properties 50-22-6, Corticosterone 50-23-7, Hydrocortisone 50-24-8, Prednisolone 50-27-1, Estratriol 50-28-2, Estradiol, properties 50-29-3, DDT, properties 50-32-8, Benzo[a]pyrene, properties 50-36-2, Cocaine 50-49-7, Imipramine 50-78-2, Aspirin 51-55-8, Atropine, properties 51-79-6, Ethyl carbamate 52-43-7 52-44-8, 2,4-Diazaspiro[5.5]undecane-1,3,5-trione 53-06-5, Cortisone 53-16-7, Estrone, properties 55-21-0, Benzamide 56-23-5, properties 56-49-5, 3-Methylcholanthrene 57-13-6, Urea, properties 57-27-2, properties 57-43-2, 5-Ethyl-5-(3-methylbutyl)barbituric acid 57-44-3, Barbital 57-83-0, Progesterone, properties 57-97-6, 7,12-Dimethylbenz[a]anthracene 58-08-2, properties 58-18-4, 17.alpha.-Methyltestosterone 58-22-0, Testosterone 58-55-9, Theophylline, properties 58-90-2, 2,3,4,6-Tetrachlorophenol 59-46-1, Procaine 60-29-7, Diethyl ether, properties 60-35-5, Acetamide, properties 60-80-0 61-82-5, 1H-1,2,4-Triazol-3-amine 62-23-7, p-Nitrobenzoic acid 62-44-2, Phenacetin 62-53-3, Benzenamine, properties 62-56-6, Thiourea, properties 63-25-2, Carbaryl 64-17-5, Ethanol, properties 64-19-7, Acetic acid, properties 64-85-7, Deoxycorticosterone 65-45-2, o-Hydroxybenzamide 65-85-0, Benzoic acid, properties 66-22-8, Uracil, properties 66-25-1, Hexanal 67-56-1, Methanol, properties 67-63-0, 2-Propanol, properties 67-66-3, Trichloromethane, properties 67-72-1, Hexachloroethane 68-96-2, 17.alpha.-Hydroxyprogesterone 69-72-7, properties 70-55-3, p-Toluenesulfonamide 71-23-8, 1-Propanol, properties 71-36-3, 1-Butanol, properties 71-41-0, 1-Pentanol, properties 71-43-2, Benzene, properties 71-55-6, 1,1,1-Trichloroethane 73-24-5, Adenine, properties 74-11-3 74-82-8, Methane, properties 74-83-9, Bromomethane, properties 74-84-0, Ethane, properties 74-85-1, Ethene, properties 74-86-2, Ethyne, properties 74-88-4, properties 74-95-3, Dibromomethane 74-96-4, Bromoethane 74-97-5, Bromochloromethane 74-98-6, Propane, properties 74-99-7, Propyne 75-00-3, Chloroethane 75-01-4, properties 75-03-6, Iodoethane 75-04-7, Ethylamine, properties 75-05-8, Acetonitrile, properties 75-08-1, Ethanethiol 75-09-2, properties 75-11-6, Diiodomethane 75-18-3, Dimethyl sulfide 75-25-2, Tribromomethane 75-26-3, 2-Bromopropane 75-27-4, Bromodichloromethane 75-28-5, 2-Methylpropane 75-29-6, 2-Chloropropane 75-30-9, 2-Iodopropane 75-34-3, 1,1-Dichloroethane 75-35-4, 1,1-Dichloroethylene,

properties 75-50-3, Trimethylamine, properties 75-52-5, properties 75-56-9, properties 75-83-2, 2,2-Dimethylbutane 75-84-3 75-85-4, 2-Methylbutan-2-ol 75-89-8, 2,2,2-Trifluoroethanol 75-97-8, 3,3-Dimethyl-2-butanone 76-01-7, Pentachloroethane 76-03-9, Trichloroacetic acid, properties 76-06-2, Chloropicrin 76-13-1, 1,1,2-Trichlorotrifluoroethane 76-14-2, 1,2-Dichlorotetrafluoroethane 76-22-2, Camphor 76-57-3, Codeine 76-73-3, Secobarbital 76-74-4, Pentobarbital 76-76-6, 5-Ethyl-5-isopropylbarbituric acid 77-02-1, 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)-5-(2-propenyl)- 77-74-7, 3-Methyl-3-pentanol 78-40-0, Triethyl phosphate 78-77-3, 1-Bromo-2-methylpropane 78-78-4, 2-Methylbutane 78-79-5, properties 78-83-1, 2-Methylpropan-1-ol, properties 78-86-4, 2-Chlorobutane 78-87-5, 1,2-Dichloropropane 78-92-2, Butan-2-ol 78-93-3, 2-Butanone, properties 79-00-5, 1,1,2-Trichloroethane 79-01-6, Trichloroethylene, properties 79-11-8, Chloroacetic acid, properties 79-20-9, Methyl acetate 79-24-3, Nitroethane 79-29-8, 2,3-Dimethylbutane 79-34-5, 1,1,2,2-Tetrachloroethane 79-41-4, Methacrylic acid, properties 79-46-9, 2-Nitropropane 81-81-2, Warfarin 83-32-9, Acenaphthene **84-65-1**, **Anthraquinone** 84-66-2, Diethyl phthalate 85-01-8, Phenanthrene, properties 85-34-7, Chlorfenac 86-57-7, 1-Nitronaphthalene 86-73-7, Fluorene 86-74-8, 9H-Carbazole 87-61-6, 1,2,3-Trichlorobenzene 87-65-0, 2,6-Dichlorophenol 87-68-3, Hexachloro-1,3-butadiene 87-85-4, Hexamethylbenzene 87-86-5, Pentachlorophenol 88-06-2, 2,4,6-Trichlorophenol 88-65-3, 2-Bromobenzoic acid 88-72-2, o-Nitrotoluene 88-73-3, o-Chloronitrobenzene 88-74-4, o-Nitroaniline 88-75-5 89-80-5, Menthone 89-83-8, Thymol 90-05-1, o-Methoxyphenol 90-11-9, 1-Bromonaphthalene 90-12-0, 1-Methylnaphthalene 90-13-1, 1-Chloronaphthalene 90-14-2, 1-Iodonaphthalene 90-15-3, 1-Naphthol 91-15-6, Phthalonitrile 91-17-8, Decalin 91-20-3, Naphthalene, properties 91-22-5, Quinoline, properties 91-23-6, o-Nitroanisole 91-57-6, 2-Methylnaphthalene 91-58-7, 2-Chloronaphthalene 91-66-7, N,N-Diethylaniline 92-24-0, Naphthacene 92-52-4, Biphenyl, properties 92-69-3, p-Phenylphenol 92-87-5, 1,1'-Biphenyl-4,4'-diamine 93-58-3, Methyl benzoate 93-89-0, Ethyl benzoate 94-09-7, Ethyl p-aminobenzoate 94-12-2, Risocaine 94-25-7, Butamben 94-82-6, 2,4-DB 95-46-5, 2-Bromotoluene 95-47-6, o-Xylene, properties 95-48-7, properties 95-49-8, 2-Chlorotoluene 95-50-1, 1,2-Dichlorobenzene 95-51-2, o-Chloroaniline 95-53-4, o-Toluidine, properties 95-55-6, o-Aminophenol 95-57-8, 2-Chlorophenol 95-63-6, 1,2,4-Trimethylbenzene 95-65-8, 3,4-Dimethylphenol 95-77-2, 3,4-Dichlorophenol **95-93-2**, 1,2,4,5-Tetramethylbenzene 95-94-3, 1,2,4,5-Tetrachlorobenzene 95-95-4, 2,4,5-Trichlorophenol 96-14-0, 3-Methylpentane 96-22-0, 3-Pentanone 96-33-3, Methyl acrylate 96-37-7, Methylcyclopentane 96-47-9, 2-Methyltetrahydrofuran 97-23-4, Dichlorophen 97-95-0, 2-Ethyl-1-butanol 97-96-1, 2-Ethylbutanal 98-01-1, Furfural, properties 98-06-6, tert-Butylbenzene 98-54-4 98-82-8, Isopropylbenzene 98-85-1, 1-Phenylethanol 98-86-2, Acetophenone,

properties 98-95-3, Nitrobenzene, properties 99-04-7, m-Toluic acid 99-08-1, 3-Nitrotoluene 99-09-2 99-35-4, 1,3,5-Trinitrobenzene 99-49-0, Carvone 99-54-7, 3,4-Dichloronitrobenzene 99-65-0, 1,3-Dinitrobenzene 99-76-3, Methylparaben 99-87-6, 4-Isopropyltoluene 99-94-5, p-Toluic acid 99-96-7, 4-Hydroxybenzoic acid, properties 99-99-0, p-Nitrotoluene 100-00-5, p-Chloronitrobenzene 100-01-6, properties 100-02-7, 4-Nitrophenol, properties 100-17-4, p-Nitroanisole 100-25-4, 1,4-Dinitrobenzene 100-41-4, Ethylbenzene, properties 100-42-5, properties 100-44-7, Benzyl chloride, properties 100-46-9, Benzylamine, properties 100-47-0, Benzonitrile, properties 100-51-6, Phenylmethanol, properties 100-52-7, Benzaldehyde, properties 100-61-8, N-Methylaniline, properties 100-66-3, Anisole, properties 100-71-0, 2-Ethylpyridine 101-42-8, Fenuron 101-81-5, Diphenylmethane 101-84-8, Diphenyl ether 102-69-2, Tripropylamine 102-76-1, Glyceryl triacetate 103-29-7, Bibenzyl 103-33-3, Azobenzene 103-65-1, Propylbenzene
(correlation and prediction of the soly. of compds. in water using an amended solvation energy relationship)

IT 103-69-5, N-Ethylaniline 103-82-2, Phenylacetic acid, properties 103-84-4, Acetanilide 103-85-5, Phenylthiourea 103-88-8, p-Bromoacetanilide 103-90-2, p-Hydroxyacetanilide 104-04-1 104-51-8, Butylbenzene 104-76-7 105-05-5, 1,4-Diethylbenzene 105-30-6, 2-Methylpentan-1-ol 105-37-3, Ethyl propionate 105-53-3, Malonic acid diethyl ester 105-54-4, Ethyl butyrate 105-57-7, 1,1-Diethoxyethane 105-66-8, Propyl butyrate 105-67-9, 2,4-Dimethylphenol 106-30-9, Ethyl heptylate 106-32-1, Ethyl octanoate 106-36-5, Propyl propanoate 106-37-6, 1,4-Dibromobenzene 106-38-7, 4-Bromotoluene 106-39-8, p-Chlorobromobenzene 106-41-2, 4-Bromophenol 106-42-3, p-Xylene, properties 106-43-4, 4-Chlorotoluene 106-44-5, properties 106-46-7, 1,4-Dichlorobenzene 106-47-8, p-Chloroaniline, properties 106-48-9, 4-Chlorophenol 106-49-0, p-Methylaniline, properties 106-70-7, Methyl hexanoate 106-93-4, 1,2-Dibromoethane 106-94-5 106-97-8, Butane, properties 106-98-9, 1-Butene, properties 106-99-0, 1,3-Butadiene, properties 107-00-6, 1-Butyne 107-04-0, 1-Chloro-2-bromoethane 107-06-2, properties 107-08-4, 1-Iodopropane 107-10-8, Propylamine, properties 107-12-0, Propionitrile 107-13-1, 2-Propenenitrile, properties 107-31-3, Methyl formate 107-83-5, 2-Methylpentane 107-87-9, 2-Pentanone 108-03-2, 1-Nitropropane 108-08-7, 2,4-Dimethylpentane 108-10-1, 4-Methyl-2-pentanone 108-11-2, 4-Methyl-2-pentanol 108-20-3, Diisopropyl ether 108-21-4, Isopropyl acetate 108-36-1, 1,3-Dibromobenzene 108-37-2, Benzene, 1-bromo-3-chloro- 108-38-3, properties 108-39-4, properties 108-42-9 108-43-0, 3-Chlorophenol 108-44-1, 3-Methylaniline, properties 108-46-3, 1,3-Benzenediol, properties 108-47-4, 2,4-Dimethylpyridine 108-48-5, 2,6-Dimethylpyridine 108-67-8, 1,3,5-Trimethylbenzene, properties 108-68-9, 3,5-Dimethylphenol 108-70-3, 1,3,5-Trichlorobenzene 108-86-1, Bromobenzene, properties 108-87-2, Methylcyclohexane 108-88-3, Toluene, properties 108-90-7, Chlorobenzene, properties

108-93-0, Cyclohexanol, properties 108-94-1, Cyclohexanone, properties 108-95-2, Phenol, properties 108-98-5, Thiophenol, properties 109-60-4, Propyl acetate 109-65-9, 1-Bromobutane 109-66-0, Pentane, properties 109-67-1, 1-Pentene 109-69-3, 1-Chlorobutane 109-73-9, Butylamine, properties 109-79-5, Butanethiol 109-87-5, Dimethoxymethane 109-89-7, Diethylamine, properties 109-92-2 109-94-4, Ethyl formate 109-99-9, properties 110-00-9, Furan 110-02-1, Thiophene 110-19-0, Isobutyl acetate 110-38-3, Ethyl decanoate 110-42-9, Methyl decanoate 110-43-0, Heptan-2-one 110-45-2, Isopentyl formate 110-53-2, 1-Bromopentane 110-54-3, Hexane, properties 110-58-7, Pentylamine 110-62-3, Pentanal 110-74-7, Propyl formate 110-81-6, Diethyl disulfide 110-82-7, Cyclohexane, properties 110-86-1, Pyridine, properties 110-91-8, Morpholine, properties 111-11-5, Methyl octanoate 111-13-7, 2-Octanone 111-25-1, 1-Bromohexane 111-26-2, Hexylamine 111-27-3, 1-Hexanol, properties 111-43-3, Dipropyl ether 111-47-7, Di-n-propyl sulfide 111-65-9, Octane, properties 111-66-0, 1-Octene 111-68-2, Heptylamine 111-70-6, 1-Heptanol 111-76-2, 2-Butoxyethanol 111-83-1, 1-Bromooctane 111-84-2, Nonane 111-86-4, 1-Octanamine 111-87-5, 1-Octanol, properties 111-92-2, Dibutylamine 112-30-1, 1-Decanol 112-40-3, Dodecane 112-53-8, 1-Dodecanol 112-72-1, 1-Tetradecanol 112-92-5, 1-Octadecanol 113-92-8, Chlorpheniramine maleate 114-26-1, Propoxur 115-07-1, 1-Propene, properties 115-11-7, properties 115-43-5, 5-Allyl-5-phenylbarbituric acid 117-81-7, Di(2-ethylhexyl)phthalate 118-74-1, Hexachlorobenzene 118-90-1, 2-Methylbenzoic acid 118-91-2, o-Chlorobenzoic acid 118-92-3, 2-Aminobenzoic acid 118-96-7, 2,4,6-Trinitrotoluene 119-61-9, Benzophenone, properties 119-64-2, 1,2,3,4-Tetrahydronaphthalene 119-65-3, Isoquinoline 120-12-7, Anthracene, properties 120-36-5, Dichlorprop 120-47-8, Ethyl-p-hydroxybenzoate 120-80-9, 1,2-Benzenediol, properties 120-82-1, 1,2,4-Trichlorobenzene 120-83-2, 2,4-Dichlorophenol 121-14-2, 2,4-Dinitrotoluene 121-44-8, properties 121-69-7, properties 121-73-3, Benzene 1-chloro-3-nitro- 121-92-6, m-Nitrobenzoic acid 122-39-4, Diphenylamine, properties 122-99-6, 2-Phenoxyethanol 123-05-7, Hexanal, 2-ethyl- 123-08-0, p-Hydroxybenzaldehyde 123-11-5, properties 123-19-3, 4-Heptanone 123-29-5, Ethyl nonanoate 123-30-8, p-Aminophenol **123-31-9**, 1,4-Benzenediol, properties 123-38-6, Propionaldehyde, properties 123-51-3, 3-Methylbutan-1-ol 123-66-0, Ethyl hexanoate 123-72-8, Butyraldehyde 123-86-4 123-92-2, Isopentyl acetate 123-96-6, 2-Octanol 124-11-8, 1-Nonene 124-18-5, Decane 124-48-1, Chlorodibromomethane 125-40-6, Butabarbital 127-18-4, Tetrachloroethylene, properties 127-19-5, N,N-Dimethylacetamide 129-00-0, Pyrene, properties 131-11-3, Dimethyl phthalate 132-64-9, Dibenzofuran 134-32-7, 1-Naphthylamine 135-01-3, 1,2-Diethylbenzene 135-19-3, 2-Naphthol, properties 137-32-6 137-58-6, Lidocaine 141-78-6, Acetic acid ethyl ester, properties 142-28-9, 1,3-Dichloropropane 142-29-0, Cyclopentene 142-62-1, Hexanoic acid, properties 142-68-7, Tetrahydropyran 142-82-5,

Heptane, properties 142-84-7, Dipropylamine 142-96-1, Dibutyl ether 143-08-8, 1-Nonanol 156-59-2, cis-1,2-Dichloroethylene 191-24-2, Benzo[ghi]perylene 192-97-2, Benzo[e]pyrene 198-55-0, Perylene 205-82-3, Benzo[j]fluoranthene 205-99-2, Benzo[b]fluoranthene 206-44-0, Fluoranthene 207-08-9, Benzo[k]fluoranthene 208-96-8, Acenaphthylene 213-46-7, Picene 217-59-4, Triphenylene 218-01-9, Chrysene 287-92-3, Cyclopentane 288-13-1, Pyrazole 291-64-5, Cycloheptane 292-64-8, Cyclooctane 299-42-3, Ephedrine 330-54-1, Diuron 330-55-2, Linuron 334-48-5, Decanoic acid 351-83-7, p-Fluoroacetanilide 352-93-2, Diethyl sulfide 372-18-9, 1,3-Difluorobenzene 437-38-7, Fentanyl 462-06-6, Fluorobenzene 464-06-2, 2,2,3-Trimethylbutane 464-07-3, 3,3-Dimethyl-2-butanol 479-23-2, Cholanthrene 496-11-7, Indan 502-41-0, Cycloheptanol 502-56-7, 5-Nonanone 513-35-9, 2-Methyl-2-butene 513-36-0, 1-Chloro-2-methylpropane 513-81-5, 2,3-Dimethyl-1,3-butadiene 526-73-8, 1,2,3-Trimethylbenzene 527-60-6, 2,4,6-Trimethylphenol 527-84-4, 2-Isopropyltoluene 528-29-0, 1,2-Dinitrobenzene 534-52-1, DNOC 535-80-8 536-75-4, 4-Ethylpyridine 538-68-1, Pentylbenzene 538-93-2, Isobutylbenzene 539-03-7, p-Chloroacetanilide 539-82-2, Ethyl pentanoate 540-36-3, 1,4-Difluorobenzene 540-54-5, 1-Chloropropane 540-84-1, 2,2,4-Trimethylpentane 541-73-1, 1,3-Dichlorobenzene 542-55-2, Isobutyl formate 542-69-8, 1-Iodobutane 543-49-7, 2-Heptanol 543-59-9, 1-Chloropentane

(correlation and prediction of the soly. of compds. in water using an amended solvation energy relationship)

L34 ANSWER 2 OF 16 HCA COPYRIGHT 2003 ACS

130:182250 Method for metal-catalyzed activation of bis(triorganosilyl) peroxides for oxidation of aromatic compounds. Teles, Joaquim Henrique; Schulz, Michael; Sundermeyer, Joerg; Jost, Carsten (BASF A.-G., Germany). Ger. Offen. DE 19736428 A1 19990225, 14 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1997-19736428 19970821.

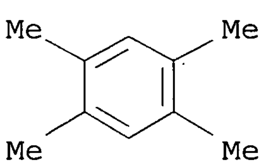
AB Arom. compds. are oxidized to **quinones** by bis(triorganosilyl) peroxides in presence of a metal acid catalyst. Thus, 2-methylnaphthalene was oxidized with Me3SiOOSiMe3 in presence of Re2O7 and Bu3PO in CHCl3 to give 59% 2-methyl-1,4-naphthoquinone and 8% 6-methyl-1,4-naphthoquinone.

IT **95-93-2, Durene**

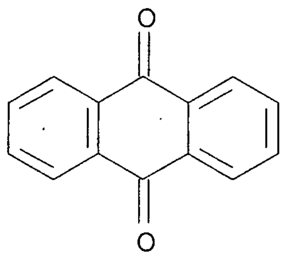
(rhenium-catalyzed oxidn. of arom. compds. with bis(triorganosilyl) peroxides)

RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **84-65-1P**, **Anthraquinone**
(rhenium-catalyzed oxidn. of arom. compds. with bis(triorganosilyl) peroxides)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



IC ICM C07C046-02
ICS C07F007-18
ICA C07C050-02; C07C050-12; C07C050-18; B01J031-22; B01J031-12; B01J031-02; B01J023-36
CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 91-57-6, 2-Methylnaphthalene 93-04-9, 2-Methoxynaphthalene **95-93-2**, **Durene** 120-12-7, Anthracene, reactions 128-39-2, 2,6-Di-tert-butylphenol 2078-54-8, 2,6-Diisopropylphenol 2416-94-6, 2,3,6-Trimethylphenol 5796-98-5, Bis(trimethylsilyl) peroxide 6443-69-2, 3,4,5-Trimethoxytoluene
(rhenium-catalyzed oxidn. of arom. compds. with bis(triorganosilyl) peroxides)
IT 58-27-5P, 2-Methyl-1,4-naphthoquinone **84-65-1P**, **Anthraquinone** 527-17-3P, Duroquinone 605-93-6P, 6-Methyl-1,4-naphthoquinone 605-94-7P, 2,3-Dimethoxy-5-methyl-p-benzoquinone 719-22-2P, 2,6-Di-tert-butyl-p-benzoquinone 935-92-2P, 2,3,5-Trimethyl-p-benzoquinone 1988-11-0P, 2,6-Diisopropyl-p-benzoquinone 2348-82-5P, 2-Methoxy-1,4-naphthoquinone
(rhenium-catalyzed oxidn. of arom. compds. with bis(triorganosilyl) peroxides)

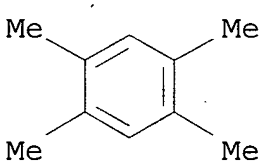
L34 ANSWER 3 OF 16 HCA COPYRIGHT 2003 ACS
128:270417 Selective C-H bond activation of arenes catalyzed by methylrhenium trioxide. Jacob, Josemon; Espenson, James H. (Ames Laboratory and Department of Chemistry, Iowa State University, Ames, IA, 50011, USA). Inorganica Chimica Acta, 270(1,2), 55-59 (English) 1998. CODEN: ICHAA3. ISSN: 0020-1693. OTHER SOURCES: CASREACT 128:270417. Publisher: Elsevier Science S.A..
AB Arenes, in glacial acetic acid, are oxidized to p-benzoquinones by hydrogen peroxide when methylrhenium trioxide (CH3ReO3 or MTO) is used as a catalyst. In some cases an intermediate **hydroquinon** was also obtained in lower yield. Oxidn. of the Me side chains of various methylbenzenes did not occur. The active catalyst species are the previously characterized .eta.2-peroxorhenium complexes, CH3Re(O)2(.eta.2-O2) and

CH3Re(O)(.eta.2-O2)2(H2O). Sep. tests showed that **hydroquinones** and phenols are oxidized by H2O2-MTO more rapidly than the simple arenes; in the proposed mechanism they are intermediate products. Higher conversions were found for the more highly-substituted arenes, consistent with their being the most reactive species toward the electrophilically active peroxide bound to rhenium. High conversions of the less substituted members of the series were not achieved, reflecting concurrent deactivation of MTO-peroxide, a process of greater import for the more slowly reacting substrates.

IT **95-93-2**, 1,2,4,5-Tetramethylbenzene
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

RN 95-93-2 HCA

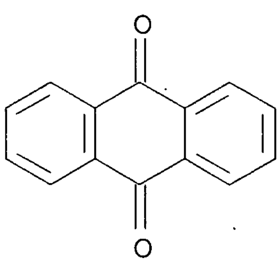
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **84-65-1P**, **Anthraquinone**
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

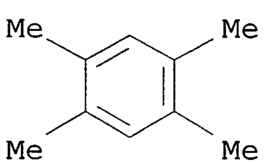
IT **Quinones**
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

IT 85-01-8, Phenanthrene, reactions 95-47-6, o-Xylene, reactions 95-48-7, 2-Methylphenol, reactions 95-63-6, 1,2,4-Trimethylbenzene **95-93-2**, 1,2,4,5-Tetramethylbenzene 106-42-3, p-Xylene, reactions 108-38-3, reactions 119-64-2, Tetralin 120-12-7, Anthracene, reactions
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

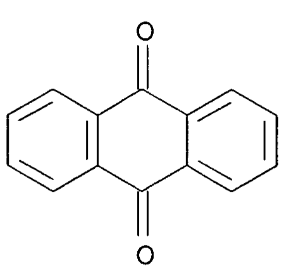
IT 527-18-4P 700-13-0P, Trimethyl-p-**hydroquinone**
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed

oxidn. of arenes)
IT 84-11-7P, Phenanthraquinone **84-65-1P**, **Anthraquinone** 137-18-8P, 2,5-Dimethyl-p-benzoquinone 526-86-3P, 2,3-Dimethyl-p-benzoquinone 527-17-3P, Tetramethyl-p-benzoquinone 527-61-7P, 2,6-Dimethyl-p-benzoquinone 553-97-9P, Methyl-p-benzoquinone 935-92-2P, Trimethyl-p-benzoquinone 7474-90-0P
(prepn. of benzoquinones by methylrhenium trioxide-catalyzed oxidn. of arenes)

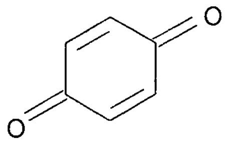
L34 ANSWER 4 OF 16 HCA COPYRIGHT 2003 ACS
118:254511 Oxidation of arenes to para-**quinones** with hydrogen peroxide catalyzed by hexafluoroacetone hydrate. Adam, Waldemar; Ganeshpure, Pralhad A. (Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Germany). Synthesis (3), 280-2 (English) 1993. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 118:254511.
AB Various arom. hydrocarbons were oxidized with aq. hydrogen peroxide in the presence of hexafluoroacetone hydrate as catalyst to give p-**quinones** and/or the ring cleavage oxidn. products. The regioselective oxidn. of 2-methylnaphthalene to 2-methyl-1,4-naphthoquinone (vitamin K3) was studied in detail.
IT **95-93-2**
(oxidn. of, with hydrogen peroxide)
RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



IT **84-65-1P**, 9,10-Anthracenedione **106-51-4P**, 2,5-Cyclohexadiene-1,4-dione, preparation
(prepn. of)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



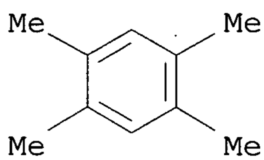
RN 106-51-4 HCA
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



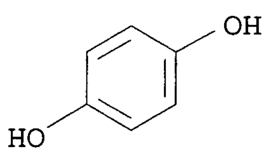
CC 25-27 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 30
ST oxidn arene; hexafluoroacetone hydrate catalyst oxidn arene; regioselective oxidn methylnaphthalene; vitamin K3; **quinone**
IT Oxidation
(of arenes with hydrogen peroxide, **quinones** by)
IT 85-01-8, Phenanthrene, reactions 91-20-3, Naphthalene, reactions 91-57-6, 2-Methylnaphthalene 93-04-9, 2-Methoxynaphthalene 95-47-6, reactions **95-93-2** 108-95-2, Phenol, reactions 120-12-7, Anthracene, reactions
(oxidn. of, with hydrogen peroxide)
IT 58-27-5P **84-65-1P**, 9,10-Anthracenedione **106-51-4P**
, 2,5-Cyclohexadiene-1,4-dione, preparation 130-15-4P, 1,4-Naphthalenedione 434-84-4P, [9,9'-Bianthracene]-10,10'(9H,9'H)-dione 526-86-3P 527-17-3P 605-93-6P 18454-53-0P 147801-91-0P 147801-92-1P
(prepn. of)

L34 ANSWER 5 OF 16 HCA COPYRIGHT 2003 ACS
117:277 Mechanism of allergic cross-reactions. I. Multispecific binding of ligands to a mouse monoclonal anti-DNP IgE antibody. Varga, Janos M.; Kalchschmid, Gertrud; Klein, Georg F.; Fritsch, Peter (Dep. Dermatol., Univ. Innsbruck, Innsbruck, 6020, Austria). Molecular Immunology, 28(6), 641-54 (English) 1991. CODEN: MOIMD5. ISSN: 0161-5890.
AB A recently developed solid-phase binding assay was used to investigate the specificity of ligand binding to a mouse monoclonal anti-dinitrophenyl IgE (I). All DNP-amino acids, that were tested inhibited the binding of the radio-labeled I to DNP covalently attached to polystyrene microplates; however, the concn. for 50% inhibition varied within four orders of magnitude, DNP-L-serine being the most and DNP-L-proline the least potent inhibitor. In addn. to DNP analogs, a large no. of drugs and other compds. were tested for their ability to compete with DNP for the binding site of I. At the concn. used for screening, 59% of compds. had no significant inhibition; 19% inhibited the binding of I more than 50%. Several families of compds. (tetracyclines, polymyxins, phenothiazines, salicylates, and **quinones**) that were effective competitors were found. Within these families, changes in the functional groups attached to the family stem had major effects on the affinity of ligand binding. The occurrence frequencies of interactions of ligands with I is in good agreement with the semi-empirical model for multispecific antibody-ligand interactions.
IT **95-93-2**, Durol **123-31-9**, **Hydroquinone**,

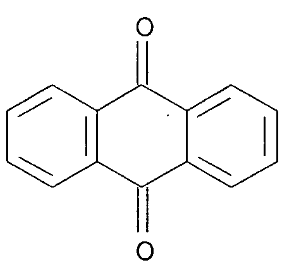
biological studies
(binding of, to anti-dinitrophenol monoclonal antibody, allergic cross-reaction mechanism in relation to)
RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



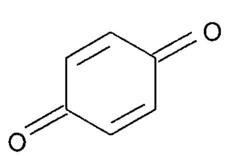
RN 123-31-9 HCA
CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



IT **84-65-1, Anthraquinone 106-51-4,**
p-Benzoquinone, biological studies
(binding of, to anti-dinitrophenol monoclonal antibody, allergic cross-reaction mechanisms in relation to)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



RN 106-51-4 HCA
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 1-3 (Pharmacology)
Section cross-reference(s): 4, 15

IT Antibiotics
Chemicals
Pharmaceuticals
Ligands
Quinones
Sulfonamides
(antibodies to dinitrophenol binding by, allergic cross-reaction mechanism in relation to)

IT 94-19-9, Globucid 94-62-2, Piperine 94-67-7 95-04-5, Ectylurea 95-15-8, Thionaphthene 95-20-5 95-48-7, biological studies 95-63-6, Pseudocumene 95-80-7 95-87-4 **95-93-2**, Durol 96-91-3 97-05-2, Sulfosalicylic acid 97-24-5 97-65-4, biological studies 98-71-5 98-79-3, 5-Oxo-L-proline 98-92-0, 3-Pyridinecarboxamide 98-96-4, Pyrazinamide 99-06-9, biological studies 99-14-9, Tricarballylic acid 99-20-7 99-26-3, Dermatol 99-50-3, 3,4-Dihydroxybenzoic acid 99-53-6, 2-Methyl-4-nitrophenol 99-76-3, Nipagin 99-93-4 99-96-7, biological studies 100-88-9 100-97-0, biological studies 101-31-5 101-38-2 101-99-5, Phenylurethane 102-08-9, Diphenylthiourea 102-98-7, Phenylmercuryborate 103-01-5, N-Phenylglycine 103-03-7, 1-Phenylsemicarbazide 103-16-2, Monobenzon 103-41-3, Cinnamic acid benzylester 103-82-2, Phenylacetic acid, biological studies 103-85-5, Phenylthiourea 103-90-2 104-15-4, biological studies 105-67-9 106-44-5, biological studies 106-48-9 106-49-0, p-Toluidine, biological studies 106-50-3, 1,4-Benzenediamine, biological studies 107-97-1, Sarcosine 108-39-4, m-Cresole, biological studies 108-45-2, 1,3-Benzenediamine, biological studies 108-73-6, Phloroglucine 109-57-9, Thiosinamine 110-44-1 110-85-0, Piperazine, biological studies 111-20-6, Decanedioic acid, biological studies 112-47-0, 1,10-Decanediol 112-72-1, Tetradecanol 112-86-7 113-22-4, Styptanon 113-52-0 113-59-7, Taractan 114-80-7 114-86-3, Phenformin 115-24-2, Sulfonal 115-33-3 115-77-5, biological studies 116-38-1, Edrophonium-chloride 117-10-2, Istizin 117-34-0, Diphenylacetic acid 117-89-5, Trifluoperazin 118-41-2, 3,4,5-Trimethoxybenzoic acid, biological studies 118-55-8, Salol 118-57-0, Salophen 118-76-3 118-79-6 118-82-1 119-39-1, 1(2H)-Phthalazinone 119-58-4 119-90-4 119-91-5, 2,2'-Biquinoline 119-93-7 120-14-9, Veratrumaldehyde 120-18-3, 2-Naphthalenesulfonic acid 120-22-9, p-Nitrosodiethylaniline 120-46-7, Dibenzoylmethane 120-57-0, Heliotropine 120-72-9, 1H-Indole, biological studies 120-78-5 120-97-8 121-57-3 121-82-4, Hexogen 122-25-8 122-39-4, Diphenylamine, biological studies 122-59-8 122-66-7 122-69-0, Styracin **123-31-9**, **Hydroquinone**, biological studies 123-47-7, Endoiodin 124-43-6, Ortizon 124-76-5, Isoborneol 124-87-8 125-13-3 125-33-7, Primidone 125-46-2 125-51-9 125-52-0, Oxyphencyclimine hydrochloride 125-64-4, Noludar 125-85-9, Parpanit 125-99-5, Pathilon 126-02-3, Cycrimine hydrochloride 126-27-2, Oxethazaine 126-52-3, Ethinamate 126-81-8, Dimedon 127-48-0, Tridione 128-13-2 129-00-0, Pyrene, biological studies 129-20-4, Tanderil 129-77-1 130-15-4, 1,4-Naphthalenedione 130-61-0 131-01-1,

Deserpidine 131-28-2 131-49-7, Angiografin 131-73-7 132-18-3 132-53-6 132-86-5, 1,3-Naphthalenediol 133-10-8 133-32-4, 1H-Indole-3-butanoic acid 133-67-5, Trichlormethiazide 134-31-6 134-71-4, Ephetonin 135-02-4 135-19-3, 2-Naphthalenol, biological studies 135-31-9 135-44-4 135-88-6 136-38-9 136-40-3, Phenazopyridine hydrochloride 136-47-0 136-72-1, Piperic acid 136-77-6, 4-Hexylresorcine 136-82-3, Metycaine 137-26-8, Thiram 137-58-6, Xylocaine 138-14-7, Desferal 138-41-0, Benzoic acid-p-sulfamide 139-33-3, Komplexon III 139-62-8 140-22-7, Diphenylcarbazide 140-64-7 141-82-2, Malonic acid, biological studies 142-63-2, Piperazine hexahydrate 143-66-8 143-67-9, Vinblastine sulfate 143-92-0, Tropenzilium bromide 144-75-2, Diasone 146-22-5, Mogadon 146-48-5, Quebrachin 146-56-5 147-24-0, Diphenhydramine hydrochloride 147-93-3, Thiosalicylic acid 147-94-4 148-24-3, 8-Quinolinol, biological studies 148-72-1, Pilocarpine nitrate 148-79-8, Thiabendazole 149-30-4, 2-Mercaptobenzthiazole 149-91-7, Gallic acid, biological studies 150-69-6 150-76-5, Hydroquinonemonomethyl ether 150-78-7 151-83-7, Methohexital 152-02-3 152-11-4, Isoptin hydrochloride 152-72-7, Sintrom 154-69-8, Pyribenzamine hydrochloride 155-09-9 155-41-9 191-48-0, Diacenaphtho[1,2-j:1',2'-l]fluoranthene 206-44-0, Fluoranthene 217-59-4, Triphenylene 288-32-4, Imidazole, biological studies 288-47-1, Thiazole 298-81-7, Meladinine 298-96-4, Triphenyl tetrazolium chloride 299-39-8 299-42-3 300-48-1 302-70-5, Mitomen 302-79-4, Tretinoin 303-25-3, Cyclizine hydrochloride 303-69-5, Dominal 304-84-7, Etamivan 306-03-6 306-07-0 306-19-4 306-21-8, Paredrine hydrobromide 314-03-4 315-80-0, Dibenzepin hydrochloride 317-34-0 318-98-9, Propranolol hydrochloride 319-89-1, Tetrahydroxyquinone 320-77-4 331-39-5 339-43-5 341-70-8 350-12-9, Sulbentin 357-66-4, Spirilene 360-68-9, Koprosterin 364-62-5, Metoclopramide 365-26-4 382-67-2 389-08-2, Nalidixic acid 390-64-7, Segontin 396-01-0 434-13-9 435-97-2, Marcoumar 439-14-5, Valium 443-48-1, Metronidazole 447-05-2, Pyridoxine phosphate 452-86-8 456-59-7, Cyclandelate 458-24-2, Fenfluramine 466-06-8, Proscillaridin 466-09-1, Uzarigenin 471-47-6, Oxamidic acid 475-25-2, Hematine 477-93-0, Dimethoxanate 479-18-5, Isophyllen 479-27-6, 1,8-Naphthalenediamine 479-92-5 480-68-2 481-06-1, Santonin 481-85-6, 2-Methyl-1,4-naphthohydroquinone 482-05-3, Diphenic acid 482-68-8, Sarpagan-10,17-diol 482-74-6 483-84-1, Flavianic acid 484-11-7, Neocuproin 484-23-1, Nepresol
(binding of, to anti-dinitrophenol monoclonal antibody, allergic cross-reaction mechanism in relation to)

IT 50-33-9, Butazolidine, biological studies 50-41-9, Clomiphene citrate 50-48-6, Amitriptylin 50-63-5, Chloroquin diphosphate 50-71-5, Alloxan 50-78-2, Acetyl salicylic acid 50-85-1, m-Cresotinic acid 51-17-2, Benzimidazole 51-35-4, Hydroxyproline 51-55-8, Atropine, biological studies 51-66-1 51-84-3, biological studies 52-90-4, Cysteine, biological studies 54-31-9, Furosemide 54-84-2 54-95-5, Cardiazole 55-56-1, Chlorhexidine 55-98-1, Busulphan 56-40-6, Glycine, biological

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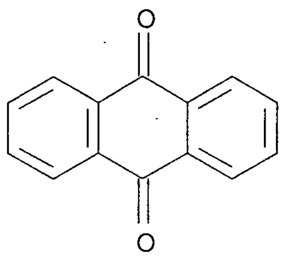
Irgafen 121-25-5, Amprolium 122-11-2, Madribon 122-80-5
124-04-9, Hexanedioic acid, biological studies 125-60-0,
Baralgin-Amid 126-07-8 126-43-2 127-69-5, Sulfafurazol
127-79-7, Sulfamerazine 127-81-1, Salthion 130-16-5 130-22-3
131-08-8 131-09-9 132-98-9, Isocillin 134-50-9,
9-Aminoacridine hydrochloride 134-81-6, Benzil 134-85-0
136-95-8, 2-Benzothiazolamine 137-08-6, Calcium-D-pantothenate
138-39-6, Mafenide 139-85-5 141-82-2, Propanedioic acid,
biological studies 143-37-3, Ethanimidamide 144-83-2 145-94-8,
Chlorindanol 146-56-5 147-24-0, Benadryl 147-55-7,
Pheneticillin 147-85-3, Proline, biological studies 148-64-1
148-82-3, Melphalan 149-15-5, Butyn Sulfate 149-64-4 150-13-0,
p-Aminobenzoic acid 150-69-6, p-Ethoxyphenylurea 152-47-6
153-61-7, Cefalotin 154-87-0, Cocarboxylase 154-97-2,
Contrathion 208-96-8, Acenaphthylene 218-01-9, Chrysene
243-42-5, Benzo[b]naphtho[2,3-d]furan 260-94-6, Acridine
298-46-4, 5H-Dibenz[b,f]azepine-5-carboxamide 298-57-7,
Cinnarizine 303-81-1, Novobiocin 305-03-3, Chlorambucil
309-00-2, Aldrin 313-67-7, Aristolochic acid 315-30-0,
Allopurinol 316-41-6, Berberinsulfate 334-48-5, Decanoic acid
346-18-9, Polythiazide 370-81-0 437-74-1 441-38-3 446-86-6,
Azathioprine 464-41-5 466-49-9, Aspidospermin 467-22-1,
Carbiphene hydrochloride 474-25-9 481-74-3 488-82-4,
D-Arabinitol 489-49-6, Cetrarin 497-76-7, Arbutin 498-23-7,
Citraconic acid 499-12-7, Aconitic acid 515-64-0, Sulfisomidine
519-87-9, Acetyldiphenylamine 520-77-4, Ethadione 521-74-4,
Broxyquinoline 526-08-9, Sulfaphenazole 529-65-7 530-43-8,
Chloromycetin palmitate 531-75-9, Aesculin 537-05-3, Acoin
537-92-8 543-24-8, N-Acetylglycine 545-93-7 547-44-4
550-81-2, Amopyroquin
(binding of, to anti-dinitrophenol monoclonal antibody, allergic cross-reaction mechanisms in relation to)

L34 ANSWER 6 OF 16 HCA COPYRIGHT 2003 ACS
112:25982 Dependence of the rate constant for intercombination electron transfer in triplet exciplexes on energy. Levin, P. P.; Pluzhnikov, P. F.; Kuz'min, V. A. (Inst. Khim. Fiz., Moscow, USSR). Khimicheskaya Fizika, 8(6), 752-61 (Russian) 1989. CODEN: KHFID9. ISSN: 0207-401X.

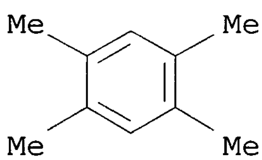
AB The rate consts. are measured by the laser photolysis method. The exciplexes arise in the quenching of the triplet states of **quinones**, arom. ketones, naphthalene nitro-derivs., and aza-arom. compds. of arom. amines and arom. hydrocarbons in various solvents. The exciplex free energies are evaluated. A correlation is found between the intercombination conversion rate consts. and the free energy of the process. The solvent reorganization energies, those of the internal degrees of freedom, and the matrix elements of the spin-orbit interaction in the exciplexes are calcd. The role of the exciplex conformation is considered for the intercombination electron transfer.

IT **84-65-1**, 9,10-**Anthraquinone 95-93-2**
106-51-4, 1,4-Benzoquinone, properties

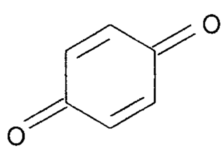
(in electron transfer in triplet exciplexes)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 106-51-4 HCA
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 22, 73
ST electron transfer triplet exciplex rate const; **quinone** electron transfer triplet exciplex; arom compd electron transfer triplet exciplex; amine arom electron transfer triplet exciplex; ketone electron transfer triplet exciplex; solvent effect electron transfer triplet exciplex
IT Ketones, properties
Quinones
(in electron transfer in triplet exciplexes)
IT 58-27-5, 2-Methyl-1,4-naphthoquinone **84-65-1**, 9,10-**Anthraquinone** 86-57-7, 1-Nitronaphthalene 87-85-4, Hexamethylbenzene 90-98-2 91-20-3, Naphthalene, properties 92-82-0, Phenazine 93-99-2 **95-93-2** 100-22-1 100-66-3, Anisole, properties **106-51-4**, 1,4-Benzoquinone, properties 118-75-2, properties 120-12-7, Anthracene, properties 130-15-4, 1,4-Naphthoquinone 260-94-6, Acridine 363-03-1, 2-Phenyl-1,4-benzoquinone 366-29-0 494-72-4 527-17-3,

Duroquinone 527-21-9 553-97-9 581-40-8, 2,3-Dimethylnaphthalene 581-42-0, 2,6-Dimethylnaphthalene 603-34-9, Triphenylamine 615-93-0, 2,5-Dichloro-1,4-benzoquinone 634-36-6, 1,2,3-Trimethoxybenzene 700-12-9, Pentamethylbenzene 701-56-4 781-43-1, 9,10-Dimethylanthracene 1207-69-8, 9-Chloroacridine 2435-53-2, Tetrachloro-1,2-benzoquinone 2887-97-0, 2,6-Diphenyl-1,4-benzoquinone 3383-21-9 3519-82-2 4985-70-0 6119-74-0, 1,4-Dimethoxy-9,10-**anthraquinone** 6932-37-2 24824-27-9, 2,7-Dinitronaphthalene 34105-76-5 69737-87-7 75552-47-5
(in electron transfer in triplet exciplexes)

L34 ANSWER 7 OF 16 HCA COPYRIGHT 2003 ACS

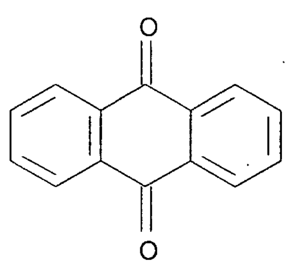
102:178452 Gas chromatographic analysis of 1,4-naphthoquinones. Nosal, A.; Skarzewski, J. (Inst. Org. Phys. Chem., Tech. Univ. Wroclaw, Wroclaw, 50-370, Pol.). Chromatographia, 20(1), 19-22 (English) 1985. CODEN: CHRGB7. ISSN: 0009-5893.

AB A gas chromatog. method is described for the anal. of 1,4-naphthoquinone derivs. in the mixts. of their isomers. The best results were obtained by using 7.5% XE-60 on Chromosorb G at 180.degree.. Quant. detn. was carried out with 1,4-naphthoquinone as the internal std. and using relative response factors or by means of the direct calibration method.

IT **84-65-1 106-51-4**, analysis
(gas chromatog. of, on Dexsil 300 and QF-1 and XE-60 stationary phases, retention in)

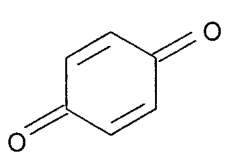
RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



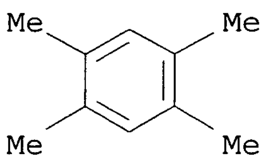
RN 106-51-4 HCA

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



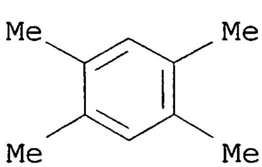
IT **95-93-2**
(sepn. of, from dimethoxytetramethylbenzene and tetramethybenzoquinone, gas chromatog.)

RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)

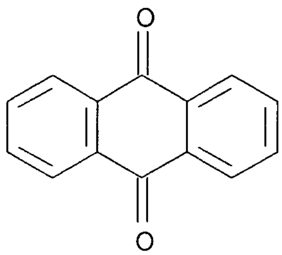


CC 80-4 (Organic Analytical Chemistry)
IT 58-27-5 **84-65-1 106-51-4**, analysis 130-15-4
482-70-2 527-17-3 605-93-6 2197-57-1 2202-79-1 2348-82-5
6290-94-4 39510-88-8 50371-31-8 81402-05-3 95931-76-3
(gas chromatog. of, on Dexsil 300 and QF-1 and XE-60 stationary phases, retention in)
IT **95-93-2**
(sepn. of, from dimethoxytetramethylbenzene and tetramethybenzoquinone, gas chromatog.)

L34 ANSWER 8 OF 16 HCA COPYRIGHT 2003 ACS
102:166431 Cerium catalyzed persulfate oxidation of polycyclic aromatic hydrocarbons to **quinones**. Skarzewski, Jacek (Inst. Org. Phys. Chem., Techn. Univ. Wroclaw, Wroclaw, 50-370, Pol.). Tetrahedron, 40(23), 4997-5000 (English) 1984. CODEN: TETRAB. ISSN: 0040-4020.
AB A practical synthesis of polycyclic **quinones** from the parent hydrocarbons is described. The two-phase oxidn. of hydrocarbons was accomplished by using ammonium persulfate in the catalytic presence of cerium ammonium sulfate, silver nitrate, and sodium dodecyl sulfate. The reaction conditions and scope have been discussed in detail. Thus, 1,4-naphthoquinone was obtained in 81% yield from naphthalene.
IT **95-93-2**
(cerium catalyzed persulfate oxidn. of)
RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)

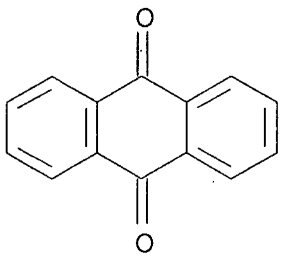


IT **84-65-1P**
(prepn. of, by oxidn. of anthracene)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)

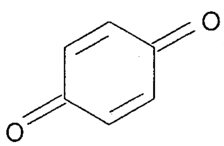


CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST polycyclic **quinone**; oxidn polycyclic hydrocarbon; naphthoquinone
IT 85-01-8, reactions 91-20-3, reactions 91-57-6 **95-93-2** 98-52-2 98-85-1 100-51-6, reactions 120-12-7, reactions 581-40-8 581-42-0 582-16-1 2506-41-4 6836-38-0 13199-54-7 35480-23-0 42101-92-8 60683-53-6
(cerium catalyzed persulfate oxidn. of)
IT **84-65-1P**
(prepn. of, by oxidn. of anthracene)
IT 4460-86-0P
(prepn. of, by oxidn. of **durene**)

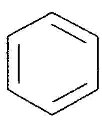
L34 ANSWER 9 OF 16 HCA COPYRIGHT 2003 ACS
102:39186 Characteristics of a thin-layer chromatogram scanner-mass spectrometer system. Ramaley, Louis; Vaughan, Margaret Anne; Jamieson, W. David (Trace Anal. Res. Cent., Dalhousie Univ., Halifax, NS, B3H 4J3, Can.). Analytical Chemistry, 57(1), 353-8 (English) 1985. CODEN: ANCHAM. ISSN: 0003-2700.
AB A novel TLC plate laser-desorption scanner interfaced with a quadrupole mass spectrometer was used to det. the response to various sample compds. spotted on different TLC surfaces. With regard to desorption characteristics, silanized silica gel provided the best results, followed by polyamide. High-performance TLC surfaces outperformed std. TLC surfaces. Best chromatogram peak shape and resoln. were obtained with silica-based surfaces. The more polar a compd., the more difficult it was to detect. Alcs. and carboxylic acids were low in sensitivity; amino acids were not detected. As mol. wt. increased and volatility decreased, detection also became more difficult. Compds. with mol. wts. > .apprx.300 could not be obsd. consistently. The method is nondestructive, plates can be rescanned or subjected to other detection methods, and does not require prior knowledge of spot size or position.
IT **84-65-1 106-51-4**, analysis **25619-60-7**
(sepn. and detection of, by thin-layer chromatog.-mass spectrometry with laser desorption plate scanner interface)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



RN 106-51-4 HCA
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 25619-60-7 HCA
CN Benzene, tetramethyl- (8CI, 9CI) (CA INDEX NAME)



4 (D1—Me)

CC 80-2 (Organic Analytical Chemistry)
IT Alcohols, analysis
Amines, analysis
Carboxylic acids, analysis
Esters, analysis
Ketones, analysis
Quinones
(sepn. and detection of, by thin-layer chromatog.-mass spectrometry with laser desorption plate scanner interface)
IT 84-62-8 **84-65-1** 84-66-2 84-74-2 90-15-3 91-01-0 92-52-4, analysis 98-86-2, analysis 99-65-0 101-84-8 102-04-5 102-82-9 103-79-7 **106-51-4**, analysis 108-46-3, analysis 109-52-4, analysis 111-11-5 111-87-5, analysis 111-92-2 112-61-8 120-80-9, analysis 122-39-4, analysis 129-00-0, analysis 130-15-4 131-11-3 142-62-1, analysis 142-96-1 151-10-0 935-50-2 25168-10-9 **25619-60-7**
(sepn. and detection of, by thin-layer chromatog.-mass

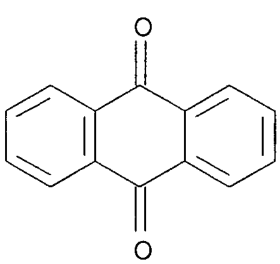
spectrometry with laser desorption plate scanner interface)

L34 ANSWER 10 OF 16 HCA
100:197286 Identification of organic compounds obtained from incineration of municipal waste by high-performance liquid chromatographic fractionation and gas chromatography-mass spectrometry. Tong, H. Y.; Shore, D. L.; Karasek, F. W.; Helland, P.; Jellum, E. (Chem. Dep., Univ. Waterloo, Waterloo, ON, N2L 3G1, Can.). Journal of Chromatography, 285(3), 423-41 (English) 1984. CODEN: JOCRAM. ISSN: 0021-9673.

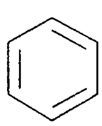
AB A gradient, normal-phase high-performance liq. chromatog. (HPLC) sepn. procedure that effectively provides a compd. class sepn. was applied to the anal. of exts. of fly ash from municipal incinerators. Each fraction collected from the HPLC procedure was analyzed by capillary gas chromatog. and capillary gas chromatog.-mass spectrometry. More than 200 org. components were identified in 1 ext. The polychlorinated dibenzodioxins (PCDDs) were exclusively eluted in 1 fraction, which facilitated their quantitation. The retention indexes of some environmentally important polychlorinated org. compds. were detd. with an av. std. deviation of 0.023. The av. recovery of the PCDD compds. in the HPLC sepn. step was 105% with a relative std. deviation of 6.8%.

IT **84-65-1 25619-60-7**
(detection of, in fly ash from municipal waste incinerators)

RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



RN 25619-60-7 HCA
CN Benzene, tetramethyl- (8CI, 9CI) (CA INDEX NAME)

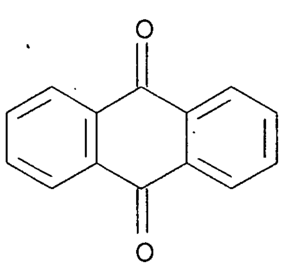


4 (D1—Me)

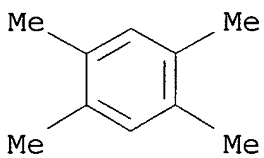
CC 60-6 (Waste Treatment and Disposal)
Section cross-reference(s): 59, 80

IT Aromatic hydrocarbons, analysis
(polycyclic, ketone and **quinone** derivs., detection of, in fly ash from municipal waste incinerators)
IT 50-32-8, analysis 58-08-2, analysis 58-90-2 65-85-0, analysis 82-05-3 82-44-0 84-15-1 **84-65-1** 84-66-2 84-74-2 85-01-8, analysis 85-68-7 88-06-2 90-12-0 90-47-1 91-20-3, analysis 91-57-6 92-06-8 92-52-4, analysis 92-94-4 93-99-2 94-41-7 103-29-7 104-72-3 117-81-7 118-74-1 129-00-0, analysis 132-64-9 132-65-0 192-97-2 203-12-3 206-44-0 208-96-8 217-59-4 218-01-9 230-17-1 479-79-8 486-25-9 571-58-4 571-61-9 575-37-1 575-41-7 575-43-9 581-40-8 581-42-0 582-16-1 608-93-5 610-48-0 613-12-7 641-96-3 643-93-6 644-08-6 829-26-5 832-64-4 832-69-9 832-71-3 883-20-5 970-06-9 1081-75-0 1081-77-2 1127-76-0 1166-18-3 1321-64-8 1335-87-1 1430-97-3 1730-37-6 1746-01-6 2051-24-3 3268-87-9 3674-74-6 5737-13-3 12002-48-1 12408-10-5 **25619-60-7** 26444-19-9 26444-20-2 26914-33-0 27554-26-3 28652-72-4 28715-26-6 28779-32-0 29446-15-9 30402-14-3 30402-15-4 30678-61-6 30746-58-8 34465-46-8 35465-71-5 35822-46-9 36088-22-9 37871-00-4 38998-75-3 39227-28-6 41593-24-2 41674-04-8 43047-99-0 43048-00-6 53742-07-7 55684-94-1 58200-70-7 64844-52-6 69760-96-9 72776-75-1 80398-28-3 85897-29-6 86006-43-1 90077-73-9 90077-74-0 90077-75-1 90077-76-2 90077-77-3 90077-78-4 90077-79-5 90077-80-8
(detection of, in fly ash from municipal waste incinerators)

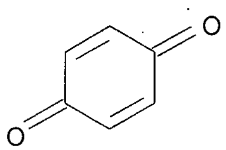
L34 ANSWER 11 OF 16 HCA COPYRIGHT 2003 ACS
100:12290 Chemical oxidizability of organic components in water.
Janicke, W. (Fed. Rep. Ger.). WaBoLu-Berichte (1), 114 pp. (German) 1983. CODEN: WBLBD6. ISSN: 0172-7702.
AB The calcd. COD values of 582 chem. compds. are compared to the COD values detd. exptl. by the Cr2O72-, Cr2O72- and Ag, and MnO4- methods.
IT **84-65-1 95-93-2 106-51-4**, biological studies **123-31-9**, properties
(COD of, exptl. and calcd. values of)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



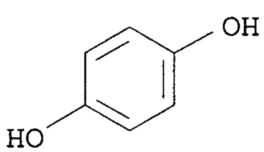
RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 106-51-4 HCA
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 123-31-9 HCA
CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



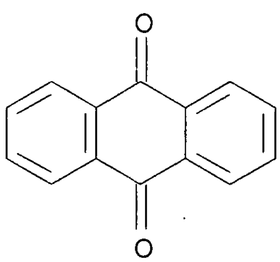
CC 61-3 (Water)
IT 50-21-5, biological studies 50-29-3, biological studies 50-71-5 50-81-7, biological studies 50-85-1 50-99-7, biological studies 51-79-6 56-12-2, biological studies 56-23-5, biological studies 56-38-2 56-40-6, properties 56-65-5, properties 56-81-5, biological studies 56-84-8, biological studies 56-86-0, biological studies 56-89-3, properties 57-09-0 57-10-3, biological studies 57-11-4, biological studies 57-13-6, properties 57-50-1, biological studies 57-88-5, properties 58-89-9 58-90-2 59-50-7 59-67-6, properties 60-00-4, biological studies 60-11-7 60-27-5 60-29-7, biological studies 60-31-1 60-33-3, biological studies 60-35-5, properties 61-90-5, biological studies 62-23-7 62-53-3, biological studies 62-55-5 62-56-6, properties 63-74-1 64-17-5, properties 64-19-7, properties 65-45-2 65-61-2 65-71-4 65-85-0, properties 66-22-8, properties 67-48-1 67-52-7 67-56-1, properties 67-63-0, biological studies 67-64-1, biological studies 67-66-3, biological studies 67-68-5, biological studies 67-71-0 67-72-1 68-11-1, biological studies 68-12-2, biological studies 69-65-8 69-72-7, biological studies 69-93-2, properties 70-18-8, properties 70-30-4 71-23-8, biological studies 71-36-3, biological studies 71-41-0, properties 71-43-2, properties 71-55-6 72-55-9, biological studies 73-22-3, biological studies 73-40-5 74-97-5 75-04-7,

biological studies 75-05-8, properties 75-08-1 75-09-2, biological studies 75-15-0, properties 75-18-3 75-25-2 75-27-4 75-34-3 75-50-3, biological studies 75-52-5, biological studies 75-65-0, biological studies 75-75-2 75-76-3 75-85-4 75-86-5 75-98-9 75-99-0 76-03-9, biological studies 76-05-1, biological studies 76-22-2 77-78-1 77-92-9, biological studies 78-10-4 78-40-0 78-59-1 78-79-5, biological studies 78-82-0 78-87-5 78-93-3, biological studies 78-95-5 79-00-5 79-01-6, biological studies 79-09-4, biological studies 79-10-7, biological studies 79-11-8, biological studies 79-20-9 79-24-3 79-31-2 79-34-5 80-62-6 81-88-9 82-68-8 83-32-9 83-33-0 84-61-7 **84-65-1** 84-66-2 84-74-2 85-01-8, properties 86-28-2 86-50-0 86-57-7 86-73-7 86-95-3 87-41-2 87-63-8 87-65-0 87-66-1 87-68-3 87-69-4, biological studies 87-86-5 88-06-2 88-72-2 88-73-3 88-74-4 88-75-5 88-89-1 88-99-3, biological studies 89-58-7 89-59-8 89-64-5 89-78-1 89-83-8 89-86-1 90-01-7 90-02-8, biological studies 90-04-0 90-05-1 90-12-0 90-15-3 90-30-2 90-43-7 90-44-8 90-64-2 91-17-8 91-20-3, properties 91-22-5, properties 91-23-6 91-66-7 92-52-4, biological studies 92-84-2 92-87-5 92-94-4 93-18-5 93-55-0 93-76-5 94-74-6 94-75-7, biological studies 94-96-2 95-15-8 95-16-9 95-47-6, biological studies 95-48-7, biological studies 95-49-8 95-50-1 95-51-2 95-53-4, biological studies 95-54-5, properties 95-65-8 95-68-1 95-76-1 95-80-7 95-85-2 95-87-4 95-92-1 **95-93-2** 95-94-3 95-95-4 96-13-9 96-33-3 96-34-4 96-41-3 97-00-7 97-05-2 97-53-0 97-54-1 97-59-6 98-00-0 98-01-1, properties 98-06-6 98-07-7 98-08-8 98-16-8 98-54-4 98-55-5 98-82-8 98-86-2, biological studies 98-95-3, biological studies 99-08-1 99-50-3 99-52-5 99-54-7 99-65-0 99-89-8 99-99-0 100-00-5 100-01-6, biological studies 100-02-7, biological studies 100-10-7 100-41-4, biological studies 100-42-5, biological studies 100-44-7, biological studies 100-47-0, properties 100-51-6, biological studies 100-52-7, properties 100-61-8, biological studies 100-63-0 100-66-3, biological studies 100-97-0, biological studies 101-81-5 101-84-8 102-07-8 102-27-2 102-71-6, biological studies 102-82-9 103-30-0 103-33-3 103-50-4 103-69-5
(COD of, exptl. and calcd. values of)

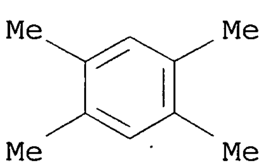
IT 103-71-9, biological studies 103-72-0 103-84-4 104-12-1 104-40-5 105-54-4 105-60-2, biological studies 106-40-1 106-42-3, biological studies 106-44-5, biological studies 106-46-7 106-47-8, properties 106-48-9 106-50-3, properties **106-51-4**, biological studies 106-89-8, biological studies 106-93-4 107-02-8, biological studies 107-05-1 107-06-2, biological studies 107-07-3, biological studies 107-11-9 107-13-1, biological studies 107-15-3, biological studies 107-19-7 107-21-1, biological studies 107-43-7 107-92-6, biological studies 107-95-9 108-05-4, biological studies 108-10-1 108-20-3 108-38-3, biological studies 108-39-4, biological studies 108-42-9 108-45-2, properties 108-70-3

108-73-6 108-75-8 108-80-5 108-86-1, properties 108-87-2 108-88-3, biological studies 108-90-7, biological studies 108-91-8, biological studies 108-93-0, properties 108-94-1, properties 108-95-2, properties 108-98-5, properties 109-43-3 109-52-4, biological studies 109-57-9 109-73-9, biological studies 109-86-4 109-89-7, biological studies 109-97-7 109-99-9, properties 110-00-9 110-02-1 110-15-6, properties 110-16-7, biological studies 110-19-0 110-44-1 110-54-3, properties 110-60-1 110-82-7, properties 110-83-8, properties 110-86-1, properties 110-88-3, properties 110-89-4, properties 110-91-8, properties 111-13-7 111-20-6, biological studies 111-26-2 111-27-3, properties 111-42-2, biological studies 111-46-6, biological studies 111-55-7 111-57-9 111-69-3 111-76-2 111-87-5, properties 112-27-6 112-30-1 112-31-2 112-34-5 112-80-1, biological studies 112-85-6 112-92-5 112-95-8 115-29-7 115-77-5, biological studies 117-81-7 118-74-1 118-91-2 118-92-3 119-33-5 119-53-9 119-61-9, biological studies 119-64-2 120-12-7, properties 120-51-4 120-61-6 120-72-9, properties 120-80-9, biological studies 120-82-1 120-83-2 121-14-2 121-44-8, biological studies 121-57-3 121-69-7, biological studies 122-14-5 122-32-7 122-39-4, properties 122-66-7 122-79-2 123-01-3 123-30-8 **123-31-9**, properties 123-42-2 123-54-6, biological studies 123-72-8 123-75-1, properties 123-86-4 123-91-1, properties 124-04-9, biological studies 124-07-2, biological studies 124-09-4, biological studies 124-18-5 124-30-1 124-40-3, biological studies 126-73-8, biological studies 127-17-3, biological studies 127-18-4, biological studies 127-27-5 128-37-0, biological studies 128-97-2 129-00-0, properties 130-22-3 130-95-0 131-11-3 131-17-9 132-64-9 134-32-7 134-81-6 135-01-3 135-19-3, biological studies 137-26-8 138-86-3 139-13-9 139-66-2 140-22-7 140-88-5 141-32-2 141-43-5, biological studies 141-53-7 141-78-6, biological studies 141-82-2, biological studies 141-97-9 142-62-1, biological studies 142-82-5, properties 142-96-1 144-49-0 144-62-7, biological studies 147-85-3, properties 148-24-3, properties 149-91-7, biological studies 150-76-5 151-21-3, biological studies 151-50-8 151-56-4, properties 206-44-0 208-96-8 218-01-9 230-27-3 260-94-6 271-89-6 288-32-4, properties 288-88-0 291-64-5 298-12-4 302-17-0 302-72-7 306-94-5 309-00-2 313-72-4 320-51-4 330-55-2 333-20-0 334-48-5 352-93-2 357-57-3 367-12-4 371-41-5 392-56-3 420-04-2 431-03-8 452-77-7 462-06-6 463-40-1 473-90-5 489-84-9 495-40-9 495-69-2 496-11-7 499-75-2 512-69-6 514-10-3 517-60-2 530-57-4 534-22-5 534-52-1 538-71-6 540-84-1 540-88-5 541-73-1 542-59-6 542-75-6 544-12-7 544-76-3 548-62-9 554-12-1 555-43-1 555-44-2 556-52-5 563-41-7 576-24-9 576-26-1 577-11-7 583-60-8 593-51-1 594-14-9 603-35-0, properties 608-93-5 615-50-9 619-08-9 622-45-7 623-37-0 623-56-3 625-38-7 626-43-7
(COD of, exptl. and calcd. values of)

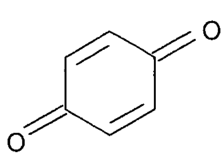
L34 ANSWER 12 OF 16 HCA COPYRIGHT 2003 ACS
93:225564 Solubility and partitioning. I: Solubility of nonelectrolytes in water. Yalkowsky, Samuel H.; Valvani, Shri C. (Pharm. Res. Unit, Upjohn Co., Kalamazoo, MI, 49001, USA). Journal of Pharmaceutical Sciences, 69(8), 912-22 (English) 1980. CODEN: JPMSAE. ISSN: 0022-3549.
AB Semiempirical anal. gave an equation that enables the estn. of the aq. soly. of either liq. or cryst. org. nonelectrolytes: log Sw .apprxeq. -1.00 log PC - 1.11[.DELTA.Sf(MP-25)/1364] + 0.54 where log PC and .DELTA.Sf are estd. from the chem. structure and MP is either known or exptl. detd. Anal. of this equation provides a means of assessing the role of crystal structure [as reflected by the m.p. (MP) and the entropy of fusion (.DELTA.Sf)] and of the activity coeff. [as reflected by the octanol-water partition coeff. (PC)] in controlling the aq. soly. of a drug. Techniques are also provided for estg. the entropy of fusion of org. compds.
IT **84-65-1 95-93-2 106-51-4**, properties
123-31-9, properties
(soly. of, calcn. of, partition in relation to)
RN 84-65-1 HCA
CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



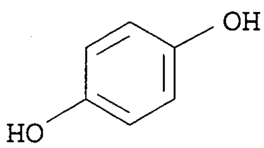
RN 95-93-2 HCA
CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 106-51-4 HCA
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 123-31-9 HCA
CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



CC 63-2 (Pharmaceuticals)
Section cross-reference(s): 22
IT 50-02-2 50-03-3 50-04-4 50-22-6 50-23-7 50-24-8 50-32-8, properties 51-79-6 52-21-1 53-06-5 56-47-3 56-49-5 56-55-3 57-10-3, properties 57-11-4, properties 57-83-0, properties 57-97-6 58-22-0 62-23-7 64-85-7 65-85-0, properties 67-78-7 71-36-3, properties 71-41-0, properties 71-43-2, properties 74-11-3 75-65-0, properties 75-84-3 75-85-4 76-03-9, properties 76-25-5 77-74-7 78-83-1, properties 78-92-2 79-11-8, properties 79-92-5 80-75-1 83-32-9 84-15-1 **84-65-1** 85-01-8, properties 86-73-7 86-74-8 87-61-6 87-85-4 88-74-4 88-75-5 89-83-8 90-12-0 90-15-3 91-20-3, properties 91-57-6 92-06-8 92-24-0 92-52-4, properties 92-94-4 94-09-7 94-12-2 94-13-3 94-25-7 94-26-8 95-50-1 **95-93-2** 95-94-3 97-95-0 99-04-7 99-05-8 99-09-2 99-76-3 99-94-5 100-00-5 100-01-6, properties 100-02-7, properties 100-25-4 102-94-3, properties 103-26-4 103-32-2 103-33-3 103-82-2, properties 104-76-7 105-30-6 106-37-6 106-38-7 106-39-8 106-41-2 106-44-5, properties 106-46-7 106-49-0, properties **106-51-4**, properties 108-11-2 108-30-5, properties 108-36-1 108-37-2 108-46-3, properties 108-70-3 108-82-7 108-86-1, properties 108-90-7, properties 108-93-0, properties 108-95-2, properties 109-57-9 110-61-2 110-94-1 111-27-3, properties 111-70-6 111-87-5, properties 112-30-1 112-37-8 112-53-8 112-72-1 112-79-8 112-92-5 112-95-8 118-74-1 118-79-6 118-90-1 118-91-2 118-92-3 118-96-7 119-61-9, properties 120-12-7, properties 120-47-8 120-80-9, properties 120-82-1 121-14-2 121-73-3 121-92-6 122-39-4, properties 122-66-7 **123-31-9**, properties 123-51-3 123-76-2 123-96-6 124-94-7 129-00-0, properties 134-32-7 134-81-6 135-19-3, properties 137-32-6 143-07-7, properties 143-08-8 150-13-0 191-24-2 198-55-0 206-44-0 217-59-4 218-01-9 238-84-6 243-17-4 302-17-0 334-48-5 367-11-3 372-18-9 378-44-9 420-04-2 462-06-6 464-07-3 495-48-7 496-11-7 501-52-0 503-64-0 523-80-8 528-29-0 535-80-8 538-56-7 540-36-3 541-73-1 543-49-7 544-63-8, properties 552-16-9 553-90-2 555-43-1 565-60-6 565-67-3 571-58-4 571-61-9 575-41-7 581-40-8 581-42-0 583-53-9 583-55-1 584-02-1 588-59-0 589-55-9 589-82-2 589-87-7 590-36-3 591-18-4 591-50-4 593-45-3 593-49-7 594-60-5 594-83-2 595-41-5 597-49-9 597-96-6 598-75-4 600-36-2 606-07-5 608-21-9

608-29-7 608-69-5 608-93-5 612-71-5 613-12-7 615-41-8
615-42-9 615-54-3 615-68-9 617-29-8 619-45-4 621-82-9,
properties 623-37-0 623-93-8 624-31-7 624-38-4 624-49-7
624-51-1 624-95-3 625-06-9 625-23-0 625-25-2 625-99-0
626-00-6 626-39-1 626-44-8 626-89-1 626-93-7 627-59-8
628-99-9 629-76-5 629-92-5 629-94-7 629-97-0 629-99-2
630-02-4 634-66-2 634-90-2 636-28-2 637-87-6 638-67-5
(soly. of, calcn. of, partition in relation to)

L34 ANSWER 13 OF 16 HCA COPYRIGHT 2003 ACS

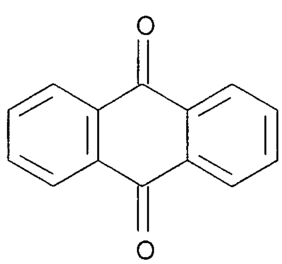
89:66360 Determination of thermal conductivity of solid organic compound in crystalline state. Wuestner, Rolf (Inst. Thermodyn., Tech. Univ. Braunschweig, Braunschweig, Fed. Rep. Ger.). Forschung im Ingenieurwesen, 44(2), 37-41 (German) 1978. CODEN: FIGWA5. ISSN: 0015-7899.

AB An app. is described for the detn. of the thermal cond. of granulated solids which are insol. in the liq. media. Data are listed for the temp. range 10-70.degree. (or to the m.p.) for anthracene, **anthraquinone**, benzene, benzil, benzophenone, benzoquinone, benzoyl peroxide, biphenyl, diphenylbutadiene, di-Ph carbonate, biphenyldicarboxylic acid, hexamethylbenzene, naphthalene, naphthoquinone, nitronaphthalene, p-quaterphenyl, trans-stilbene, terephthalaldehyde, di-Me terephthalate, o- and p-terphenyl, tetramethylbenzene, 1,2,3- and 1,3,5-trichlorobenzene, and triphenylmethane. The values are compared of the thermal cond. of Teflon obtained by this method in which a thin cylindrical sample is used.

IT **84-65-1 106-51-4**, properties **25619-60-7**
(thermal cond. of)

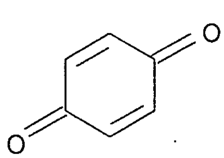
RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)

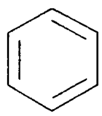


RN 106-51-4 HCA

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



RN 25619-60-7 HCA
CN Benzene, tetramethyl- (8CI, 9CI) (CA INDEX NAME)



4 (D1—Me)

CC 69-2 (Thermodynamics, Thermochemistry, and Thermal Properties)
ST cond thermal org solid app; anthracene thermal cond; **anthraquinone** thermal cond; benzene thermal cond; benzil thermal cond; benzophenone thermal cond; benzoquinone thermal cond; benzyl peroxide thermal cond; biphenyl thermal cond; methylbenzene thermal cond; naphthalene thermal cond; naphthoquinone thermal cond; nitronaphthalene thermal cond; quaterphenyl thermal cond; stilbene thermal cond; terephthalaldehyde thermal cond; terphenyl thermal cond; chlorobenzene thermal cond; phenylmethane thermal cond; butadiene diphenyl thermal cond; carbonate diphenyl thermal cond; biphenyldicarboxylic acid thermal cond; terephthalate dimethyl thermal cond; teflon thermal cond
IT 71-43-2, properties 84-15-1 **84-65-1** 87-61-6 87-85-4 91-20-3, properties 92-52-4, properties 92-94-4 94-36-0, properties 102-09-0 103-30-0 **106-51-4**, properties 108-70-3 119-61-9, properties 120-12-7, properties 120-61-6 130-15-4 134-81-6 135-70-6 519-73-3 623-27-8 886-65-7 9002-84-0 **25619-60-7** 27254-36-0 51317-27-2
(thermal cond. of)

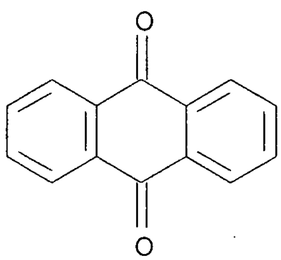
L34 ANSWER 14 OF 16 HCA COPYRIGHT 2003 ACS
80:132581 Formation of charge-transfer complexes by solid state reaction. Electronic spectra and relative reactivity. Sato, Hiroyasu; Yasuniwa, Tamiharu (Coll. Lib. Arts, Kagoshima Univ., Kagoshima, Japan). Bulletin of the Chemical Society of Japan, 47(2), 368-72 (English) 1974. CODEN: BCSJA8. ISSN: 0009-2673.
AB Formation of charge-transfer complexes by solid state reaction was studied for 16 donors; e.g. hexamethylbenzene, naphthalene, and 10 acceptors, e.g., tetracyclomethylene, p-benzoquinone. The relative reactivity of 160 pairs was detd. by the presence or absence of the charge-transfer band or grinding the component pairs of the same concentration (dild. with NaCl) for the same length of time. Equil. was not reached within the grinding time. This relative reactivity had a parallel relation with the relative ease of formation of the charge-transfer complex on evaporating a mixt. of the solns. of components, indicating that the relative reactivity was related to an apparent equil. established on the grain surface. Relative reactivity was dependent on mol. size and geometry. Smaller mols. were more reactive. For mols. with the same no. of rings, those

with compact structure were more reactive. Most of the new bands given by the reaction were charge-transfer (CT) bands of microcrystals. A fairly good linear relation was found between the transition energies of the CT bands and the ionization potentials of the donors or the electron affinities of the acceptors.

IT **84-65-1 95-93-2 106-51-4**, reactions
(charge-transfer complexes of, in solid state)

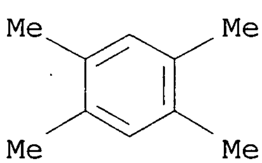
RN 84-65-1 HCA

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)



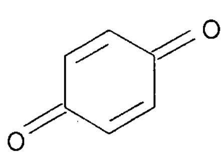
RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 106-51-4 HCA

CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)

IT 84-58-2 **84-65-1** 85-01-8, reactions 87-85-4 89-32-7 91-20-3, reactions 92-24-0 92-52-4, reactions 92-94-4 **95-93-2** 100-22-1 **106-51-4**, reactions 117-08-8 118-75-2, reactions 120-12-7, reactions 129-00-0, reactions 130-15-4 135-70-6 198-55-0 217-59-4 218-01-9 366-29-0 571-61-9 615-93-0 670-54-2, reactions 1518-16-7
(charge-transfer complexes of, in solid state)

L34 ANSWER 15 OF 16 HCA COPYRIGHT 2003 ACS

57:69996 Original Reference No. 57:13980h-i,13981a Antioxidant efficiency versus structure. Banm, Bernard; Perun, A. L. (Union

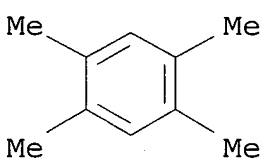
Carbide Plastics Co., Bound Brook, NJ). SPE Transactions, 2, 250-7 (Unavailable) 1962. CODEN: SPETA8. ISSN: 0096-8129.

AB The behavior in polyethylene of 76 antioxidants of different structures was investigated. These included phenols, thiobisphenols, aryl amines, other N- and S-containing stabilizers. The mechanisms underlying the action of each class of additives were considered. The phenolic and amine antioxidants appear to function primarily through chain termination and chain transfer. The metal salts of dithiocarbamates and dithiophosphates, which were effective at high temp., probably function by ionically decompg. polymer hydroperoxides. It is likely that more than one mechanism may apply to the same compd. under different use conditions.

IT **95-93-2**, Benzene, 1,2,4,5-tetramethyl- **106-51-4**, p-Benzoquinone
    (as antioxidant in ethylene polymers)

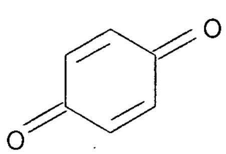
RN 95-93-2 HCA

CN Benzene, 1,2,4,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 106-51-4 HCA

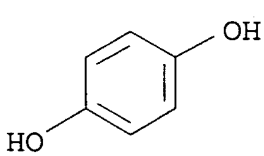
CN 2,5-Cyclohexadiene-1,4-dione (9CI) (CA INDEX NAME)



IT **123-31-9**, **Hydroquinone**
    (as antioxidant, in ethylene polymers)

RN 123-31-9 HCA

CN 1,4-Benzenediol (9CI) (CA INDEX NAME)



CC 47 (Plastics)

IT 57-13-6, Urea 82-46-2, **Anthraquinone**, 1,5-dichloro- 83-07-8, Antipyrine, 4-amino- 83-32-9, Acenaphthene 83-56-7, 1,5-Naphthalenediol 87-51-4, Indole-3-acetic acid 87-87-6, **Hydroquinone**, tetrachloro- 91-60-1, 2-Naphthalenethiol

91-64-5, Coumarin 95-55-6, Phenol, o-amino- **95-93-2**, Benzene, 1,2,4,5-tetramethyl- 96-65-1, o-Cresol, 4,4'-methylenebis[6-tert-butyl- 97-74-5, Sulfide, bis(dimethylthiocarbamoyl) 98-54-4, Phenol, p-tert-butyl- 100-22-1, p-Phenylenediamine, N,N,N',N'-tetramethyl- 102-07-8, Carbanilide 102-08-9, Carbanilide, thio- 102-60-3, 2-Propanol, 1,1',1'',1'''-(ethylenedinitrilo)tetra- 103-85-5, Urea, 1-phenyl-2-thio- 103-96-8, p-Phenylenediamine, N,N'-bis(1-methylheptyl)- 106-50-3, p-Phenylenediamine **106-51-4**, p-Benzoquinone 110-16-7, Maleic acid 111-88-6, 1-Octanethiol 115-77-5, Pentaerythritol 117-12-4, **Anthraquinone**, 1,5-dihydroxy- 117-97-5, Zinc, bis[(pentachlorophenyl)thio]- 119-84-6, Hydrocoumarin 119-90-4, Benzidine, 3,3'-dimethoxy- 120-54-7, Tetrasulfide, bis(piperidinothiocarbonyl) 120-72-9, Indole 120-78-5, Benzothiazole, 2,2'-dithiobis- 122-66-7, Hydrazobenzene 124-22-1, Dodecylamine 126-00-1, Valeric acid, 4,4-bis(p-hydroxyphenyl)- 132-53-6, 1-Naphthol, 2-nitroso- 132-65-0, Dibenzothiophene 135-57-9, Benzanilide, 2',2'''-dithiobis- 137-26-8, Disulfide, bis(dimethylthiocarbamoyl) 141-07-1, Urea, 1,3-bis(methoxymethyl)- 149-30-4, 2-Benzothiazolethiol 150-76-5, Phenol, p-methoxy- 150-78-7, Benzene, p-dimethoxy- 489-01-0, Phenol, 2,6-di-tert-butyl-4-methoxy- 519-73-3, Methane, triphenyl- 534-52-1, o-Cresol, 4,6-dinitro- 569-42-6, 1,8-Naphthalenediol 571-60-8, 1,4-Naphthalenediol 583-46-0, Hydantoin, 5-benzylidene-2-thio- 598-04-9, Butyl sulfone 603-34-9, Triphenylamine 608-71-9, Phenol, pentabromo- 620-92-8, Phenol, 4,4'-methylenedi- 623-13-2, Sulfide, methyl p-tolyl 629-45-8, Butyl disulfide 1166-52-5, Gallic acid, dodecyl ester 1205-91-0, **Hydroquinone**, diacetate 2168-93-6, Butyl sulfoxide 2425-77-6, 1-Decanol, 2-hexyl- 2536-91-6, Benzothiazole, 2-amino-6-methyl- 2677-32-9, 2,6-Xylenol, .alpha.,.alpha.'-bis(o-hydroxyphenyl)- 3122-21-2, Succinonitrile, tetraphenyl- 3236-63-3, p-Cresol, 2,2'-methylenedi- 3419-34-9, Isopropyl potassium phosphorodithioate, (C3H7O)2(KS)PS 5384-21-4, 2,6-Xylenol, 4,4'-methylenedi- 7605-98-3, Phenol, 2,2'-thiobis[3,5-dichloro- 13288-70-5, 2,6-Xylenol, 4,4'-sulfonyldi- 14086-38-5, Stearic acid, p-aminophenyl ester 14324-55-1, Zinc, bis(diethyldithiocarbamato)- 14362-12-0, Phenol, 2,2'-methylenebis[4,6-di-tert-butyl- 16284-89-2, Carbamic acid, dimethyldithio-, selenium salt 18907-31-8, Zinc, bis(2-benzothiazolethiolato)- 19779-03-4, Phenol, 2,4,6-tris[2-(dimethylamino)ethyl]- 25103-58-6, tert-Dodecyl mercaptan 25377-76-8, Thiazoline-2-thiol 32955-04-7, Carbamic acid, diethyldithio-, lead salt 34464-51-2, Carbamic acid, diethyldithio-, bismuth salt 86428-80-0, 1,3,2-Dioxaphosphorinane, 5,5-diethyl-2-mercapto-, 2-sulfide 90114-42-4, Guanidine, diphenyl- 92576-96-0, Phenol, 2,2'-thiobis[5-chloro- 97001-20-2, Propionic acid, 3-mercapto-2-methyl-, methyl ester, S-ester with cyclic O,O-2,2-diethyltrimethylene phosphorodithioate 97692-30-3, 2,6-Xylenol, .alpha.,.alpha.'-bis(2-hydroxy-5-tert-pentylphenyl)-4-

tert-pentyl- 97723-66-5, Succinic acid, mercapto-, diethyl ester, S-ester with cyclic O,O-2,2-diethyltrimethylene phosphorodithioate 98864-59-6, Guanidine, triphenyl- 98878-54-7, p-Toluenesulfonanilide, 4',4'''-iminobis-
(as antioxidant in ethylene polymers)

IT 68-11-1, Acetic acid, mercapto- 74-31-7, p-Phenylenediamine, N,N'-diphenyl- 77-92-9, Citric acid 87-66-1, Pyrogallol 88-27-7, p-Cresol, 2,6-di-tert-butyl-.alpha.-(dimethylamino)- 88-58-4, **Hydroquinone**, 2,5-di-tert-butyl- 89-65-6, Araboascorbic acid 90-15-3, 1-Naphthol 106-44-5, p-Cresol 108-73-6, Phloroglucinol 108-95-2, Phenol 120-80-9, Pyrocatechol 123-30-8, Phenol, p-amino- **123-31-9**, **Hydroquinone** 135-19-3, 2-Naphthol 583-39-1, 2-Benzimidazolethiol 732-26-3, Phenol, 2,4,6-tri-tert-butyl-
(as antioxidant, in ethylene polymers)

L34 ANSWER 16 OF 16 HCA COPYRIGHT 2003 ACS

48:60374 Original Reference No. 48:10693g-i,10694a-g Synthesis of polymethylnaphthalenes. Abadir, B. J.; Cook, J. W.; Gibson, D. T. (Univ. Glasgow, UK). J. Chem. Soc. 8-17 (Unavailable) 1953.

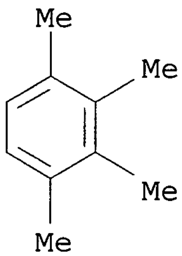
AB **Durene** (I) and 2,3-dimethylsuccinic anhydride (II) added in small portions to a stirred suspension of AlCl3 in CS2, kept overnight, the solvent decanted, and the residue decompd. with ice and HCl, washed, and recrystd. yielded 2,3,4,5-Me4C6HCOCHMeCHMeCO2H (III), m. 151-2.degree. (Me ester, m. 88.degree.; unsatd. lactone, m. 114.5.degree.), and the 2,3,5,6-tetra-Me isomer (IV), m. 147-8.degree. (Me ester, m. 103.degree.; unsatd. lactone, m. 119.degree.). III and IV with NaOBr at 100.degree. gave 2,3,4,5- and 2,3,5,6-Me4C6HCO2H, resp. Heating III or IV in a sealed tube with concd. HCl 5 hrs. at 100.degree. gave prehnitene (V) and I, resp. Friedel-Crafts reaction of V with II yields III and an isomeric acid, m. 167-8.degree.. Clemmensen reduction on III failed, while reduction with Cu chromite at 240.degree. and 130 atm. gave on working up 2,3-dimethyl-4-prehnitylbutyrolactone, m. 131-2.degree. and 2,3,4,5-Me4C6HCH2CHMeCHMeCO2H (VI), m. 135-6.degree.. VI kept in HF 30 hrs. gave 1,2,3,4-tetrahydro-1-oxo-2,3,5,6,7,8-hexamethylnaphthalene (VII), m. 120.degree., also prepd. by converting VI into the acid chloride and then treating with AlCl3 in C6H6. VII with HNO3 in a sealed tube at 175.degree. is converted to mellitic acid. VII hydrogenated with Adams catalyst in HOAc and the resulting alc. dehydrated by distn. in vacuo or treatment with HCO2H, yielded 5,6-dihydro-1,2,3,4,6,7-hexamethylnaphthalene, m. 117.degree., which was dehydrogenated with 20% Pd-C at 200-20.degree. to 1,2,3,4,6,7-C10H2Me6 (VIII), m. 145.degree. (picrate, m. 190.5.degree.; 1,3,5-C6H3(NO2)3 complex, m. 215.degree.; 2,4,7-trinitro-9-fluorenone complex, m. 210.degree.). Wolff-Kishner reduction of VII gave 5,6,7,8-tetrahydro-1,2,3,4,6,7-hexamethylnaphthalene, m. 111.degree., which on dehydrogenation gave VIII. VII treated with MeMgI in Et2O, hydrolyzed, dehydrated with HCO2H, and dehydrogenated with Pd-C yielded 1,2,3,4,5,6,7-heptamethylnaphthalene (IX), m. 134.degree. (picrate, m. 134.degree.; 1,3,5-C6H3(NO2)3 complex, m. 210.degree.;

2,4,7-trinitro-9-fluorenone complex, m. 212.degree.; styphnate, m. 168.degree.). HCl passed into a suspension of paraformaldehyde in HOAc until soln. was complete, IX added, and the suspension shaken 24 hrs., yielded on working up 8-chloromethyl-1,2,3,4,5,6,7-heptamethylnaphthalene [1,3,5-C6H3(NO2)3 complex, m. 160.degree. (decompn.)] which with 20% Pd-C in cyclohexane gave octamethylnaphthalene (X), m. 174.degree. [picrate, m. 193.degree.; 1,3,5-C6H3(NO2)3 complex, m. 192-3.degree.; 2,4,7-trinitro-9-fluorenone complex, m. 209.degree.; maleic anhydride adduct, m. 176-8.degree. (decompn.)]. The Me ester of III added to excess MeMgI and the mixt. boiled 60 hrs. in C6H6 yielded X on working up with NH4Cl and purification through the 2,4,7-trinitro-9-fluorenone complex. Friedel-Crafts reaction of V with methylsuccinic anhydride gave 2,3,4,5-Me4C6HCOCH2CHMeCO2H, m. 130-1.degree. (Et ester, m. 68.5.degree.), which on Clemmensen reduction gave 2,3,4,5-Me4C6HCH2CH2CHMeCO2H (XI), m. 106-7.degree.. XI with HF gave 1,2,3,4-tetrahydro-1-oxo-2,5,6,7,8-pentamethylnaphthalene (XII), m. 78.5.degree., which could be hydrogenated to the alc. and dehydrated to 7,8-dihydro-1,2,3,4,6-pentamethylnaphthalene, m. 64.degree., and dehydrogenated to 1,2,3,4,6-C10H3Me6 (XIII), m. 85.degree. (picrate, m. 176.degree.; 1,3,5-C6H3(NO2)3 complex, m. 187.degree.; 2,4,7-trinitro-9-fluorenone complex, m. 174.degree.; maleic anhydride, m. 138-9.degree.). XII treated with MeMgI, hydrolyzed, dehydrated, and dehydrogenated yielded 1,2,3,4,5,6-C10H2Me6, m. 81.5.degree. (picrate, m. 167-8.degree.; 1,3,5-C6H3(NO2)3 complex, m. 186.degree.; 2,4,7-trinitro-9-fluorenone complex, m. 181.degree.; maleic anhydride adduct, m. 134-6.degree.). Chloromethylation of XIII, followed by reduction with Pd-C and H, gave 1,2,3,4,5,7-C10HMe7 (XV), m. 140.degree. (picrate, m. 188.degree.; 1,3,5-C6H3(NO2)3 complex, m. 207.degree.; 2,4,7-trinitro-9-fluorenone complex, m. 199.degree.), which on further chloromethylation and reduction gave IX. (CMeClEt)2 (XIV) added during 2 hrs. to a stirred mixt. of .omicron.-xylene and AlCl3, and the mixt. kept 6 hrs. at 40.degree., was decompd. with ice and HCl, dried, and distd. yielded XV and VIII. Condensation of XIV with V at 35-40.degree. followed by heating with Se yielded VIII, IX, and X. The same condensation carried out at 60.degree. gave hexamethylanthracene, m. 236-7.degree. (picrate, m. 214.degree.; 1,3,5-C6H3(NO2)3 complex, m. 224.degree.; 2,4,7-trinitro-9-fluorenone complex, m. 228.degree.; hexamethylanthraquinone, m. 199.degree.). Condensation of p-xylene with [CHMeC(OH)Me2]2 (XVI) and AlCl3 gave 1,2,4-trimethylanthracene, m. 244.degree. (**quinone**, m. 162-3.degree.). The ultraviolet absorption spectra of the polymethylnaphthalenes are reported.

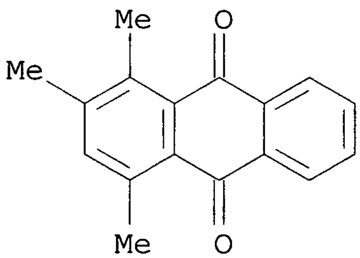
IT **488-23-3**, Benzene, 1,2,3,4-tetramethyl- **20153-30-4**
, **Anthraquinone**, 1,2,4-trimethyl-
(prepn. of)

RN 488-23-3 HCA

CN Benzene, 1,2,3,4-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 20153-30-4 HCA
CN 9,10-Anthracenedione, 1,2,4-trimethyl- (9CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)
IT 1(2H)-Naphthalenone, 3,4-dihydro-2,3,5,6,7,8-hexamethyl-
1,4-Ethenonaphthalene-2,3-dicarboxylic anhydride, 1,2,3,4-tetrahydro-1,4,5,6,7,8,9,10-octamethyl-
1,4-Ethenonaphthalene-2,3-dicarboxylic anhydride, 1,2,3,4-tetrahydro-1,4,5,6,9,10-hexamethyl-
1,4-Ethenonaphthalene-2,3-dicarboxylic anhydride, 1,2,3,4-tetrahydro-1,4,6,7,9,10-hexamethyl-
3-Butenoic acid, 4-hydroxy-2,3-dimethyl-4-[2,3,4,5-tetramethylphenyl]-, .gamma.-lactones
3-Butenoic acid, 4-hydroxy-2,3-dimethyl-4-[2,3,5,6-tetramethylphenyl]-, .gamma.-lactones
Anthraquinone, hexamethyl-
Butyric acid, 2,3-dimethyl-4-(2,3,4,5-tetramethylphenyl)-
Butyric acid, 2-methyl-3-[2,3,4,5-tetramethylbenzoyl]-
Butyric acid, 2-methyl-3-[2,3,4,5-tetramethylbenzoyl]-, methyl esters
Butyric acid, 2-methyl-3-[2,3,5,6-tetramethylbenzoyl]-
Butyric acid, 2-methyl-3-[2,3,5,6-tetramethylbenzoyl]-, methyl esters
Naphthalene, 1,2-dihydro-2,3,5,6,7,8-hexamethyl-
Naphthalene, 1-(chloromethyl)-2,3,4,5,6,7,8-heptamethyl-, compd. with 1,3,5-trinitrobenzene
Naphthalene, 5,6-dihydro-1,2,3,4,7-pentamethyl-
Propionic acid, 2-methyl-3-(2,3,4,5-tetramethylbenzoyl)-, ethyl ester
IT **488-23-3**, Benzene, 1,2,3,4-tetramethyl- 2529-39-7, Benzoic acid, 2,3,4,5-tetramethyl- 2604-45-7, Benzoic acid,

2,3,5,6-tetramethyl- **20153-30-4**, **Anthraquinone**,
1,2,4-trimethyl- 62571-58-8, Naphthalene, 1-(chloromethyl)-
2,3,4,5,6,7,8-heptamethyl- 101499-24-5, Propionic acid,
2-methyl-3-(2,3,4,5-tetramethylbenzoyl)- 107203-94-1,
1(2H)-Naphthalenone, 3,4-dihydro-2,5,6,7,8-pentamethyl-
108667-47-6, Butyric acid, 2-methyl-4-(2,3,4,5-tetramethylphenyl)-
412321-24-5, Naphthalene, 1,2,3,4-tetrahydro-2,3,5,6,7,8-hexamethyl-
(prepn. of)